



ROMÂNIA
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RECTORATUL

Universitatea Babeș-Bolyai Competiția Excelenței 2010

Dosar individual

Notă: Toate datele se referă la perioada 2005-2009

Nume, prenume, grad did.	BEU TITUS-ADRIAN, PROF. DR.
Facultatea, Catedra	Fizică
Domeniul științific	Fizică teoretică și computațională
Adresa paginii web personale	http://phys.ubbcluj.ro/~titus.beu/
Adresa e-mail	titus.beu@phys.ubbcluj.ro

Criteria I - Output - pondere 60%

2573.0

1. Articole științifice publicate în reviste indexate ISI

2473.0

Se acorda 30 puncte pentru fiecare articol si se tine cont de numărul de autori.

Formula de calcul: $(30 / \text{număr de autori}) \times \text{Factor de impact ISI} \times 10$

ISI Web of Knowledge

Cumulated IF / author: 8.771

Sum of Times Cited: 296

Average Citations per Item: 8.46

H-index: 12

Record 1

Author(s): Diudea, MV (Diudea, Mircea V.); Vizitiu, AE (Vizitiu, Aniela E.); Beu, T (Beu, Titus); Bende, A (Bende, Attila); Nagy, CL (Nagy, Csaba L.); Janezic, D (Janezic, Dusanka)

Title: Circulene covered fullerenes

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 904 (1-3): 28-34 JUN 30 2009

Times Cited: 0

IF / autor: $1.167 / 6 = 0.195$

Punctaj: $300 \times 1.167 / 6 = 58.35$

Record 2

Author(s): Beu, TA (Beu, Titus A.); Horvath, L (Horvath, Lorand); Ghisoiu, I (Ghisoiu, Ioan)

Title: Tight-binding molecular dynamics simulations of radiation-induced C-60 fragmentation

Source: PHYSICAL REVIEW B, 79 (5): Art. No. 054112 FEB 2009

Times Cited: 0

IF / autor: $3.322 / 3 = 1.107$

Punctaj: $300 \times 3.322 / 3 = 332.2$

Record 3

Author(s): Horvath, L (Horvath, Lorand); Beu, TA (Beu, Titus A.)

Title: Tight-binding molecular dynamics simulations of radiation-induced fragmentation of C-60

Source: PHYSICAL REVIEW B, 77 (7): Art. No. 075102 FEB 2008

Times Cited: 3

IF / autor: $3.172 / 2 = 1.586$

Punctaj: $300 \times 3.172 / 2 = 475.8$

Record 4

Author(s): Beu, TA (Beu, Titus A.); Onoe, J (Onoe, Jun)

Title: First-principles calculations of the vibrational spectra of one-dimensional C-60 polymers

Source: PHYSICAL REVIEW B, 74 (19): Art. No. 195426 NOV 2006

Times Cited: 3

IF / autor: $3.107 / 2 = 1.554$

Punctaj: $300 \times 3.107 / 2 = 466.1$

Record 5

Author(s): Steinbach, C (Steinbach, Christof); Buck, U (Buck, Udo); Beu, TA (Beu, Titus A.)

Title: Infrared spectroscopy of large ammonia clusters as a function of size

Source: JOURNAL OF CHEMICAL PHYSICS, 125 (13): Art. No. 133403 OCT 7 2006

Times Cited: 5

IF / autor: $3.166 / 3 = 1.055$

Punctaj: $300 \times 3.166 / 3 = 316.6$

Record 6

Author(s): Beu, TA

Title: Simulations of biological ion channels by molecular dynamics

Source: JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS, 8 (1): 160-163 FEB 2006

Times Cited: 0

IF / autor: $1.106 / 1 = 1.106$

Punctaj: $300 \times 1.106 / 1 = 331.8$

Record 7

Author(s): Beu, TA

Title: Electronic structure calculations of peanut-shaped C-60 polymers

Source: JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS, 8 (1): 177-180 FEB 2006

Times Cited: 0

IF / autor: $1.106 / 1 = 1.106$

Punctaj: $300 \times 1.106 / 1 = 331.8$

Record 8

Author(s): Beu, TA; Onoe, J; Hida, A

Title: First-principles calculations of the electronic structure of one-dimensional C-60 polymers

Source: PHYSICAL REVIEW B, 72 (15): Art. No. 155416 OCT 2005

Times Cited: 13

IF / autor: $3.185 / 3 = 1.062$

Punctaj: $300 \times 3.185 / 3 = 318.5$

2. Articole științifice publicate în ISI proceedings

Se acorda 30 puncte pentru fiecare articol si se tine cont de numărul de autori.

Formula de calcul: $(30 / \text{număr de autori}) \times \text{Factor de impact ISI} \times 10$

In cazul in care nu are Factor de impact ISI

Se acorda 20 puncte pentru fiecare articol si se tine cont de numărul de autori.

Formula de calcul: $20 / \text{număr de autori}$

1. T. A. Beu,
"Efficient electrolyte modeling in MD simulations of transport in membrane channels",

XX Sitges Conference, Physical Biology: from Molecular Interactions to Cellular Behavior, 5-9 June 2006, Sitges, Barcelona, Spain, pp.90-91.

2. T. A. Beu,
"Efficient electrolyte modeling in MD simulations of bulk liquids, interfaces and ion channels",
CCP2007, Conference on Computational Physics, Brussels, 5-8 September 2007, Université Libre de Bruxelles, Editor Michel Mareschal, pp 325.
3. T. A. Beu,
"Simulations of radiation induced fragmentation of C60 fullerenes",
Modeling and Simulation of New Materials, Proceedings of Modeling and Simulation of New Materials: Tenth Granada Lectures, Granada, Spain, 15-19 September 2008, Series: AIP Conference Proceedings, Vol. 1091, Editors: Pedro L Garrido, Pablo I. Hurtado, and Joaquín Marro, ISBN: 978-0-7354-0624-7, 2009, pp. 249-252.

3. Articole științifice publicate în reviste indexate în BDI (din lista CNCSIS) și în reviste românești recunoscute de CNCSIS tip B și B+

40

Se acorda 10 puncte pentru fiecare articol si se tine cont de numărul de autori.

Formula de calcul: $10 / \text{număr de autori}$

1. T. A. Beu, J. Onoe, A. Hida,
"First-principles calculations of the electronic structure of one-dimensional C60 polymers",
Virtual Journal of Nanoscale Science & Technology - October 31, Volume 12, Issue 18 (2005).
Punctaj: $10 / 2 = 5$
2. T. A. Beu, J. Onoe
"First-principles calculations of the vibrational spectra of one-dimensional C60 polymers",
Virtual Journal of Nanoscale Science & Technology - December 4, Volume 14, Issue 23 (2006).
Punctaj: $10 / 2 = 5$
3. L. Horvath, T. A. Beu,
"Tight-binding molecular dynamics simulations of radiation-induced fragmentation of C60",
Virtual Journal of Nanoscale Science & Technology - February 18, Volume 17, Issue 7 (2008).
Punctaj: $10 / 2 = 5$
4. T. A. Beu, L. Horvath, I. Ghisoiu,
"Tight-binding molecular dynamics simulations of radiation-induced C60 fragmentation",
Virtual Journal of Nanoscale Science & Technology - March 9, Volume 19, Issue 10 (2009).
Punctaj: $10 / 2 = 5$
5. T. A. Beu and A.-M. Florescu,
"Revised equilibrium structures of small water clusters",
Studia Universitatis Babes-Bolyai, Physica, (2006).
Punctaj: $10 / 2 = 5$
6. T. A. Beu and A.-M. Florescu,
"Infrared spectrum calculations for small water clusters",
Studia Universitatis Babes-Bolyai, Physica, (2006).
Punctaj: $10 / 2 = 5$
7. L. Horvath and T. A. Beu,
"Tight-binding molecular dynamics simulations of radiation induced fragmentation of C60",
Studia Universitatis Babes-Bolyai, Physica, (2007).
Punctaj: $10 / 2 = 5$
8. T. A. Beu, G. Cabău
"Infrared Spectroscopy of Small Water Clusters",
Studia Universitatis Babes-Bolyai, Physica, LIII, 83-87 (2008).
Punctaj: $10 / 2 = 5$

4. Alte articole științifice/capitole publicate în reviste/volume cu referenți (peer-reviewed)

Se acorda 5 puncte pentru fiecare lucrare si se tine cont de numărul de autori.

Formula de calcul: $5 / \text{număr de autori}$

5. Cărți științifice publicate în edituri internaționale

Formula de calcul: număr de pagini / număr de autori

6. Cărți științifice publicate în edituri naționale acreditate

Se acorda 20 puncte pentru fiecare 100 pagini si se tine cont de numărul de autori.

Formula de calcul: $[(\text{număr de pagini} / 100) \times 20] / \text{număr de autori}$

7. Editor de volume publicate în edituri naționale și internaționale

• edituri naționale

Se acorda 15 puncte pentru fiecare 100 pagini și se ține cont de numărul de editori.

Formula de calcul: $[(\text{număr de pagini} / 100) \times 15] / \text{număr de editori}$

• edituri internaționale

Se acorda 30 puncte pentru fiecare 100 pagini și se ține cont de numărul de editori.

Formula de calcul: $[(\text{număr de pagini} / 100) \times 30] / \text{număr de editori}$

8. Brevete internaționale

Se acorda 20 puncte pentru fiecare brevet.

Formula de calcul: $20 / \text{număr de autori}$

9. Brevete naționale

Se acorda 10 puncte pentru fiecare brevet și se ține cont de numărul de autori.

Formula de calcul: $10 / \text{număr de autori}$

10. Impact tehnologic al brevetelor: resurse financiare extrabugetare atrase în relație cu economia

Formula de calcul: $\text{valoarea în RON} / 10.000$

11. Realizări artistice naționale și internaționale (Domeniul Arte)

(Expoziții, spectacole, concerte, publicații, filme, înregistrări)

Criteriul II – Prestigiu profesional – pondere 30%

2009.4

1. Citări ale articolelor ISI listate la Criteriul I

150

Formula de calcul: $\text{număr citări} \times 10 \times \text{factor impact ISI al revistei în care este publicat articolul citat}$

Pentru articolele din reviste cu FI ISI < 1, se aplica formula de la punctul 2.

Record 3

Author(s): Horvath, L (Horvath, Lorand); Beu, TA (Beu, Titus A.)

Title: Tight-binding molecular dynamics simulations of radiation-induced fragmentation of C-60

Source: PHYSICAL REVIEW B, 77 (7): Art. No. 075102 FEB 2008

Times Cited: 3

IF: 3.172

Punctaj citări: $10 \times 1 = 10$

Citation 1

Author(s): Li, HJ (Li, Hongjian); Tang, H (Tang, Hong); Dou, YS (Dou, Yusheng)

Title: Laser-induced nonthermal fragmentation of C60 studied by semiclassical dynamics simulation

Source: MOLECULAR PHYSICS, 107 (19): 2039-2044 2009

Record 5

Author(s): Steinbach, C (Steinbach, Christof); Buck, U (Buck, Udo); Beu, TA (Beu, Titus A.)

Title: Infrared spectroscopy of large ammonia clusters as a function of size

Source: JOURNAL OF CHEMICAL PHYSICS, 125 (13): Art. No. 133403 OCT 7 2006

Times Cited: 5

IF: 3.166

Punctaj citări: $10 \times 5 = 50$

Citation 1

Author(s): Lubombo, C (Lubombo, C.); Curotto, E (Curotto, E.); Barral, PEJ (Barral, Paula E. Janeiro); Mella, M (Mella, Massimo)

Title: Thermodynamic properties of ammonia clusters (NH₃)_n n=2-11: Comparing classical and quantum simulation results for hydrogen bonded species

Source: JOURNAL OF CHEMICAL PHYSICS, 131 (3): Art. No. 034312 JUL 21 2009

Citation 2

Author(s): Sigurbjornsson, OF (Sigurbjoernsson, Omar F.); Firanescu, G (Firanescu, George); Signorell, R (Signorell, Ruth)

Title: Intrinsic Particle Properties from Vibrational Spectra of Aerosols
Source: ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 60: 127-146 2009

Citation 3

Author(s): Slipchenko, MN (Slipchenko, Mikhail N.); Sartakov, BG (Sartakov, Boris G.); Vilesov, AF (Vilesov, Andrey F.)
Title: Evolution of the vibrational spectrum of ammonia from single molecule to bulk
Source: JOURNAL OF CHEMICAL PHYSICS, 128 (13): Art. No. 134509 APR 7 2008

Citation 4

Author(s): Lane, JR (Lane, Joseph R.); Vaida, V (Vaida, Veronica); Kjaergaard, HG (Kjaergaard, Henrik G.)
Title: Calculated electronic transitions of the water ammonia complex
Source: JOURNAL OF CHEMICAL PHYSICS, 128 (3): Art. No. 034302 JAN 21 2008

Citation 5

Author(s): Slipchenko, MN (Slipchenko, Mikhail N.); Sartakov, BG (Sartakov, Boris G.); Vilesov, AF (Vilesov, Andrey F.); Xantheas, SS (Xantheas, Sotiris S.)
Title: Study of NH stretching vibrations in small ammonia clusters by infrared spectroscopy in the droplets and ab initio Calculations
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (31): 7460-7471 AUG 9 2007

Record 8

Author(s): Beu, TA; Onoe, J; Hida, A

Title: First-principles calculations of the electronic structure of one-dimensional C-60 polymers

Source: PHYSICAL REVIEW B, 72 (15): Art. No. 155416 OCT 2005

Times Cited: 13

IF: 3.185

Punctaj citări: 10 x 9 = 90

Citation 1

Author(s): Vehvilainen, TT (Vehvilainen, T. T.); Ganchenkova, MG (Ganchenkova, M. G.); Nieminen, RM (Nieminen, R. M.)
Title: C-20 Based Polymers: Electronic and Elastic Properties and Stability Studies
Source: JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY, 9 (7): 4360-4366 Sp. Iss. SI JUL 2009

Citation 2

Author(s): Shima, H (Shima, Hiroyuki); Yoshioka, H (Yoshioka, Hideo); Onoe, J (Onoe, Jun)
Title: Geometry-driven shift in the Tomonaga-Luttinger exponent of deformed cylinders
Source: PHYSICAL REVIEW B, 79 (20): Art. No. 201401 MAY 2009

Citation 3

Author(s): Ganchenkova, MG (Ganchenkova, M. G.); Vehvilainen, TT (Vehvilainen, T. T.); Nieminen, RM (Nieminen, R. M.)
Title: Quasigraphite: Density functional theory based predictions of a structure and its properties
Source: PHYSICAL REVIEW B, 78 (19): Art. No. 195421 NOV 2008

Citation 4

Author(s): Onoe, J (Onoe, Jun); Ito, T (Ito, Takahiro); Kimura, S (Kimura, Shin-ichi)
Title: Time dependence of the electronic structure of an electron-beam-irradiated C-60 film
Source: JOURNAL OF APPLIED PHYSICS, 104 (10): Art. No. 103706 NOV 15 2008

Citation 5

Author(s): Li, JL (Li, Jiling); Xia, YY (Xia, Yueyuan); Zhao, MW (Zhao, Mingwen); Liu, XD (Liu, Xiangdong); Song, C (Song, Chen); Li, LJ (Li, Lijuan); Li, F (Li, Feng); Huang, BD (Huang, Boda)
Title: Theoretical prediction for the (AlN)₁₂ fullerene-like cage-based nanomaterials
Source: JOURNAL OF PHYSICS-CONDENSED MATTER, 19 (34): Art. No. 346228 AUG 29 2007

Citation 6

Author(s): Li, JL (Li Ji-Ling); Xia, YY (Xia Yue-Yuan); Zhao, MW (Zhao Ming-Wen); Liu, XD (Liu Xiang-Dong); Song, C (Song Chen); Li, LJ (Li Li-Juan); Li, F (Li Feng); Huang, BD (Huang Bo-Da)
Title: Polymerization of silicon-doped heterofullerenes: an ab initio study
Source: CHINESE PHYSICS LETTERS, 25 (1): 246-249 JAN 2008

Citation 7

Author(s): Nakayama, H (Nakayama, Hiroyuki); Ono, T (Ono, Tomoya); Goto, H (Goto, Hidekazu); Hirose, K (Hirose, Kikuji)
Title: Electronic structures of peanut-shaped fullerene tubes
Source: SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS, 8 (3): 196-199 APR 2007

Citation 8

Author(s): Wang, Y (Wang, Yin); Zhuang, J (Zhuang, Jun); Ma, MZ (Ma, Mei-Zhong); Ning, XJ (Ning, Xi-Jing)

Title: C72 (or C120) cluster growth from C-36 (or C-60) clusters

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 807 (1-3): 201-206 APR 1 2007

Citation 9

Author(s): Fukui, K (Fukui, Ken-Ichi); Sakai, M (Sakai, Motoyoshi)

Title: Formation of one-dimensional C-60 rows on TiO₂(110)-1x2-cross-link structure and their local polymerization

Source: JOURNAL OF PHYSICAL CHEMISTRY B, 110 (42): 21118-21123 OCT 26 2006

2. Alte citări ale lucrărilor listate mai sus

Formula de calcul: număr citări x 10

3. Citări în perioada 2005-2009 ale articolelor anterioare**1060**

Formula de calcul: număr citări x 10 x factor impact ISI al revistei în care este publicat articolul citat.

Pentru articolele din reviste cu FI ISI < 1, se aplica formula de la punctul 2.

Record 9

Author(s): Steinbach, C; Andersson, P; Kazimirski, JK; Buck, U; Buch, V; Ben, TA

Title: Infrared predissociation spectroscopy of large water clusters: A unique probe of cluster surfaces

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 108 (29): 6165-6174 JUL 22 2004

Times Cited: 33

IF: 2.639

Punctaj citări: 10 x 31 = 310

Citation 1

Author(s): Sun, Q (Sun, Qiang)

Title: The Raman OH stretching bands of liquid water

Source: VIBRATIONAL SPECTROSCOPY, 51 (2): 213-217 NOV 10 2009

Citation 2

Author(s): Elango, M (Elango, M.); Subramanian, V (Subramanian, V.); Sathyamurthy, N (Sathyamurthy, N.)

Title: Structure and stability of spiro-cyclic water clusters

Source: JOURNAL OF CHEMICAL SCIENCES, 121 (5): 839-848 SEP 2009

Citation 3

Author(s): Sun, Q (Sun, Qiang); Zheng, HF (Zheng, Haifei)

Title: Raman OH stretching vibration of ice I-h

Source: PROGRESS IN NATURAL SCIENCE, 19 (11): 1651-1654 NOV 10 2009

Citation 4

Author(s): Mizuse, K (Mizuse, Kenta); Hamashima, T (Hamashima, Toru); Fujii, A (Fujii, Asuka)

Title: Infrared Spectroscopy of Phenol-(H₂O)(n > 10): Structural Strains in Hydrogen Bond Networks of Neutral Water Clusters

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 113 (44): 12134-12141 NOV 5 2009

Citation 5

Author(s): Matsuoka, H (Matsuoka, Hideto); Sekiguchi, S (Sekiguchi, Shinji); Yagi, N (Yagi, Naoto); Inoue, K (Inoue, Katsuaki); Ohta, N (Ohta, Noboru); Suzuki, T (Suzuki, Toshinori)

Title: Pneumatic Atomization of Liquid Water and Characterization of Submicrometer-Sized Droplets by Fourier Transform Infrared Spectroscopy

Source: JOURNAL OF PHYSICAL CHEMISTRY C, 113 (32): 14110-14113 AUG 13 2009

Citation 6

Author(s): Sigurbjornsson, OF (Sigurbjoernsson, Omar F.); Firanesco, G (Firanesco, George); Signorell, R (Signorell, Ruth)

Title: Intrinsic Particle Properties from Vibrational Spectra of Aerosols

Source: ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 60: 127-146 2009

Citation 7

Author(s): Prell, JS (Prell, James S.); Williams, ER (Williams, Evan R.)

Title: Structures of Thermal, Mass-Selected Water Clusters Probed with Hydrophobic Ion Tags and Infrared Photodissociation Spectroscopy

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 131 (11): 4110-4119 MAR 25 2009

Citation 8

Author(s): Wang, L (Wang, Lu); Zhao, JJ (Zhao, Jijun); Li, FY (Li, Fengyu); Fang, HP (Fang, Haiping); Lu, JP (Lu, Jian Ping)

Title: First-Principles Study of Water Chains Encapsulated in Single-Walled Carbon Nanotube
Source: JOURNAL OF PHYSICAL CHEMISTRY C, 113 (14): 5368-5375 APR 9 2009

Citation 9

Author(s): Abu-Samha, M (Abu-samha, M.); Borve, KJ (Borve, K. J.); Winkler, M (Winkler, M.); Harnes, J (Harnes, J.); Saethre, LJ (Saethre, L. J.); Lindblad, A (Lindblad, A.); Bergersen, H (Bergersen, H.); Ohrwall, G (Ohrwall, G.); Bjorneholm, O (Bjorneholm, O.); Svensson, S (Svensson, S.)
Title: The local structure of small water clusters: imprints on the core-level photoelectron spectrum
Source: JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, 42 (6): Art. No. 055201 MAR 28 2009

Citation 10

Author(s): Abu-Samha, M (Abu-Samha, M.); Borve, KJ (Borve, K. J.); Winkler, M (Winkler, M.); Harnes, J (Harnes, J.); Saethre, LJ (Saethre, L. J.); Lindblad, A (Lindblad, A.); Bergersen, H (Bergersen, H.); Ohrwall, G (Ohrwall, G.); Bjorneholm, O (Bjorneholm, O.); Svensson, S (Svensson, S.)
Title: The local structure of small water clusters: imprints on the core-level photoelectron spectrum
Source: JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS, 42 (5): Art. No. 055201 MAR 14 2009

Citation 11

Author(s): Bako, I (Bako, Imre); Megyes, T (Megyes, Tuende); Balint, S (Balint, Szabolcs); Grosz, T (Grosz, Tamas); Chihaiia, V (Chihaiia, Viorel)
Title: Water-methanol mixtures: topology of hydrogen bonded network
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 10 (32): 5004-5011 2008

Citation 12

Author(s): Abu-Samha, M (Abu-samha, M.); Borve, KJ (Borve, K. J.)
Title: Surface relaxation in water clusters: Evidence from theoretical analysis of the oxygen 1s photoelectron spectrum
Source: JOURNAL OF CHEMICAL PHYSICS, 128 (15): Art. No. 154710 APR 21 2008

Citation 13

Author(s): Tasic, U (Tasic, Uros); Day, BS (Day, B. Scott); Yan, TY (Yan, Tianying); Morris, JR (Morris, John R.); Hase, WL (Hase, William L.)
Title: Chemical dynamics study of intrasurface hydrogen-bonding effects in gas-surface energy exchange and accommodation
Source: JOURNAL OF PHYSICAL CHEMISTRY C, 112 (2): 476-490 JAN 17 2008

Citation 14

Author(s): Matsumoto, Y (Matsumoto, Yoshiteru); Honma, K (Honma, Kenji)
Title: NH stretching vibrations of pyrrole clusters studied by infrared cavity ringdown spectroscopy
Source: JOURNAL OF CHEMICAL PHYSICS, 127 (18): Art. No. 184310 NOV 14 2007

Citation 15

Author(s): Mitsui, M (Mitsui, Masaaki); Nakajima, A (Nakajima, Atsushi)
Title: Formation of large molecular cluster anions and elucidation of their electronic structures
Source: BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN, 80 (6): 1058-1074 JUN 15 2007

Citation 16

Author(s): Levering, LM (Levering, Lori M.); Sierra-Hernandez, MR (Sierra-Hernandez, M. Roxana); Allen, HC (Allen, Heather C.)
Title: Observation of hydronium ions at the air - Aqueous acid interface: Vibrational spectroscopic studies of aqueous HCl, HBr, and HI
Source: JOURNAL OF PHYSICAL CHEMISTRY C, 111 (25): 8814-8826 JUN 28 2007

Citation 17

Author(s): Mizuse, K (Mizuse, Kenta); Fujii, A (Fujii, Asuka); Mikami, N (Mikami, Naohiko)
Title: Long range influence of an excess proton on the architecture of the hydrogen bond network in large-sized water clusters
Source: JOURNAL OF CHEMICAL PHYSICS, 126 (23): Art. No. 231101 JUN 21 2007

Citation 18

Author(s): Suhara, K (Suhara, Ken-ichiro); Fujii, A (Fujii, Asuka); Mizuse, K (Mizuse, Kenta); Mikami, N (Mikami, Naohiko); Kuo, JL (Kuo, Jer-Lai)
Title: Compatibility between methanol and water in the three-dimensional cage formation of large-sized protonated methanol-water mixed clusters
Source: JOURNAL OF CHEMICAL PHYSICS, 126 (19): Art. No. 194306 MAY 21 2007

Citation 19

Author(s): Wang, ZH (Wang, Zhaohui); Pang, YS (Pang, Yoonsoo); Diott, DD (Diott, Dana D.)
Title: Hydrogen-bond disruption by vibrational excitations in water
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (17): 3196-3208 MAY 3 2007

Citation 20

Author(s): Sun, Q (Sun Qiang); Zheng, HF (Zheng Hai-Fei)
Title: Liquid water structure from anomalous density under ambient condition

Source: CHINESE PHYSICS LETTERS, 23 (11): 3022-3024 NOV 2006

Citation 21

Author(s): Wang, ZH (Wang, Zhaohui); Pang, Y (Pang, Yoonsoo); Dlott, DD (Dlott, Dana D.)

Title: Long-lived interfacial vibrations of water

Source: JOURNAL OF PHYSICAL CHEMISTRY B, 110 (41): 20115-20117 OCT 19 2006

Citation 22

Author(s): Firanescu, G (Firanescu, George); Hermsdorf, D (Hermsdorf, Dana); Ueberschaer, R (Ueberschaer, Roman); Signorell, R (Signorell, Ruth)

Title: Large molecular aggregates: from atmospheric aerosols to drug nanoparticles

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8 (36): 4149-4165 2006

Citation 23

Author(s): Gopalakrishnan, S; Liu, DF; Allen, HC; Kuo, M; Shultz, MJ

Title: Vibrational spectroscopic studies of aqueous interfaces: Salts, acids, bases, and nanodrops

Source: CHEMICAL REVIEWS, 106 (4): 1155-1175 APR 2006

Citation 24

Author(s): Farnik, M; Weimann, M; Steinbach, C; Buck, U; Borho, N; Adler, TB; Suhm, MA

Title: Size-selected methyl lactate clusters: fragmentation and spectroscopic fingerprints of chiral recognition

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8 (10): 1148-1158 MAR 14 2006

Citation 25

Author(s): Signorell, R; Jetzki, M; Kunzmann, M; Ueberschaer, R

Title: Unraveling the origin of band shapes in infrared spectra of N₂O-(CO₂)-C-12 and (CO₂)-C-12-(CO₂)-C-13 ice particles

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 110 (9): 2890-2897 MAR 9 2006

Citation 26

Author(s): Steinbach, C; Buck, U

Title: Vibrational spectroscopy of size-selected sodium-doped water clusters

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 110 (9): 3128-3131 MAR 9 2006

Citation 27

Author(s): Tyrode, E; Johnson, CM; Kumpulainen, A; Rutland, MW; Claesson, PM

Title: Hydration state of nonionic surfactant monolayers at the liquid/vapor interface: Structure determination by vibrational sum frequency spectroscopy

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 127 (48): 16848-16859 DEC 7 2005

Citation 28

Author(s): Tarbuck, TL; Richmond, GL

Title: Adsorption of organosulfur species at aqueous surfaces: Molecular bonding and orientation

Source: JOURNAL OF PHYSICAL CHEMISTRY B, 109 (44): 20868-20877 NOV 10 2005

Citation 29

Author(s): Ohno, K; Okimura, M; Akai, N; Katsumoto, Y

Title: The effect of cooperative hydrogen bonding on the OH stretching-band shift for water clusters studied by matrix-isolation infrared spectroscopy and density functional theory

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 7 (16): 3005-3014 2005

Citation 30

Author(s): Pak, C; Lee, HM; Kim, JC; Kim, D; Kim, KS

Title: Theoretical investigation of normal to strong hydrogen bonds

Source: STRUCTURAL CHEMISTRY, 16 (3): 187-202 JUN 2005

Citation 31

Author(s): Fujii, A; Enomoto, S; Miyazaki, M; Mikami, N

Title: Morphology of protonated methanol clusters: An infrared spectroscopic study of hydrogen bond networks of H⁺(CH₃OH)_n (n=4-15)

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 109 (1): 138-141 JAN 13 2005

Record 10

Author(s): Beu, TA; Steinbach, C; Buck, U

Title: Model analysis of the fragmentation of large H₂O and NH₃ clusters based on MD simulations

Source: EUROPEAN PHYSICAL JOURNAL D, 27 (3): 223-229 DEC 2003

Times Cited: 4

IF: 1.612

Punctaj citări: 10 x 2 = 20

Citation 1

Author(s): Germann, TC (Germann, T. C.)

Title: Large-scale molecular dynamics simulations of hyperthermal cluster impact

Source: INTERNATIONAL JOURNAL OF IMPACT ENGINEERING, 33 (1-12): 285-293 DEC 2006

Citation 2

Author(s): Steinbach, C; Buck, U

Title: Ionization potentials of large sodium doped ammonia clusters

Source: JOURNAL OF CHEMICAL PHYSICS, 122 (13): Art. No. 134301 APR 1 2005

Record 12

Author(s): Beu, TA; Steinbach, C; Buck, U

Title: Intermolecular vibrations of large ammonia clusters from helium atom scattering

Source: JOURNAL OF CHEMICAL PHYSICS, 117 (7): 3149-3159 AUG 15 2002

Times Cited: 8

IF: 2.998

Punctaj citări: 10 x 5 = 50

Citation 1

Author(s): Lubombo, C (Lubombo, C.); Curotto, E (Curotto, E.); Barral, PEJ (Barral, Paula E. Janeiro); Mella, M (Mella, Massimo)

Title: Thermodynamic properties of ammonia clusters (NH₃)(n) n=2-11: Comparing classical and quantum simulation results for hydrogen bonded species

Source: JOURNAL OF CHEMICAL PHYSICS, 131 (3): Art. No. 034312 JUL 21 2009

Citation 2

Author(s): Sigurbjornsson, OF (Sigurbjoernsson, Omar F.); Firanescu, G (Firanescu, George); Signorell, R (Signorell, Ruth)

Title: Intrinsic Particle Properties from Vibrational Spectra of Aerosols

Source: ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 60: 127-146 2009

Citation 3

Author(s): Lindblad, A (Lindblad, A.); Bergersen, H (Bergersen, H.); Pokapanich, W (Pokapanich, W.); Tchapyguine, M (Tchapyguine, M.); Ohrwall, G (Ohrwall, G.); Bjorneholm, O (Bjorneholm, O.)

Title: Charge delocalization dynamics of ammonia in different hydrogen bonding environments: free clusters and in liquid water solution

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 11 (11): 1758-1764 2009

Citation 4

Author(s): Firanescu, G (Firanescu, George); Luckhaus, D (Luckhaus, David); Signorell, R (Signorell, Ruth)

Title: Size effects in the infrared spectra of NH₃ ice nanoparticles studied by a combined molecular dynamics and vibrational exciton approach

Source: JOURNAL OF CHEMICAL PHYSICS, 125 (14): Art. No. 144501 OCT 14 2006

Citation 5

Author(s): Firanescu, G (Firanescu, George); Hermsdorf, D (Hermsdorf, Dana); Ueberschaer, R (Ueberschaer, Roman); Signorell, R (Signorell, Ruth)

Title: Large molecular aggregates: from atmospheric aerosols to drug nanoparticles

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8 (36): 4149-4165 2006

Record 13

Author(s): Beu, TA; Onoe, J; Takeuchi, K

Title: Structural and vibrational properties Of C-36 and its oligomers (C-36)(M=2,3,4) by tight-binding molecular dynamics

Source: EUROPEAN PHYSICAL JOURNAL D, 17 (2): 205-212 NOV 2001

Times Cited: 7

IF: 1.583

Punctaj citări: 10 x 1 = 10

Citation 1

Author(s): Lu, X; Chen, ZF

Title: Curved Pi-conjugation, aromaticity, and the related chemistry of small fullerenes (< C-60) and single-walled carbon nanotubes

Source: CHEMICAL REVIEWS, 105 (10): 3643-3696 OCT 2005

Record 14

Author(s): Beu, TA; Buck, U

Title: Structure of ammonia clusters from n=3 to 18

Source: JOURNAL OF CHEMICAL PHYSICS, 114 (18): 7848-7852 MAY 8 2001

Times Cited: 21

IF: 3.147

Punctaj citări: 10 x 13 = 130

Citation 1

Author(s): Lubombo, C (Lubombo, C.); Curotto, E (Curotto, E.); Barral, PEJ (Barral, Paula E. Janeiro); Mella, M (Mella, Massimo)

Title: Thermodynamic properties of ammonia clusters (NH₃)_n (n=2-11): Comparing classical and quantum simulation results for hydrogen bonded species

Source: JOURNAL OF CHEMICAL PHYSICS, 131 (3): Art. No. 034312 JUL 21 2009

Citation 2

Author(s): Kikuta, Y (Kikuta, Yoko); Ishimoto, T (Ishimoto, Takayoshi); Nagashima, U (Nagashima, Umpei)

Title: Deuterium-substituted water-ammonia mixed trimer clusters, (H₂O)_(n-3)(NH₃)_n (n=0,1,2,3): Interaction energy, hydrogen bond structures, and Mulliken population

Source: CHEMICAL PHYSICS, 354 (1-3): 218-224 DEC 10 2008

Citation 3

Author(s): Janeiro-Barral, PE (Janeiro-Barral, Paula E.); Mella, M (Mella, Massimo); Curotto, E (Curotto, E.)

Title: Structure and energetics of ammonia clusters (NH₃)_n (n=3-20) investigated using a rigid-polarizable model derived from ab initio calculations

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 112 (13): 2888-2898 APR 3 2008

Citation 4

Author(s): Slipchenko, MN (Slipchenko, Mikhail N.); Sartakov, BG (Sartakov, Boris G.); Vilesov, AF (Vilesov, Andrey F.); Xantheas, SS (Xantheas, Sotiris S.)

Title: Study of NH stretching vibrations in small ammonia clusters by infrared spectroscopy in the droplets and ab initio Calculations

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (31): 7460-7471 AUG 9 2007

Citation 5

Author(s): Rapacioli, M (Rapacioli, Mathias); Calvo, F (Calvo, Florent); Joblin, C (Joblin, Christine); Parneix, P (Parneix, Pascal); Spiegelman, F (Spiegelman, Fernand)

Title: Vibrations and thermodynamics of clusters of polycyclic aromatic hydrocarbon molecules: The role of internal modes

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (16): 2999-3009 APR 26 2007

Citation 6

Author(s): Janeiro-Barral, PE (Janeiro-Barral, Paula E.); Mella, M (Mella, Massimo)

Title: Study of the structure, energetics, and vibrational properties of small ammonia clusters (NH₃)_n (n=2-5) using correlated ab initio methods

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 110 (39): 11244-11251 OCT 5 2006

Citation 7

Author(s): Slipchenko, MN; Kuyanov, KE; Sartakov, BG; Vilesov, AF

Title: Infrared intensity in small ammonia and water clusters

Source: JOURNAL OF CHEMICAL PHYSICS, 124 (24): Art. No. 241101 JUN 28 2006

Citation 8

Author(s): Dong, F; Heinbuch, S; Rocca, JJ; Bernstein, ER

Title: Dynamics and fragmentation of van der Waals clusters: (H₂O)_n, (CH₃OH)_n, and (NH₃)_n upon ionization by a 26.5 eV soft x-ray laser

Source: JOURNAL OF CHEMICAL PHYSICS, 124 (22): Art. No. 224319 JUN 14 2006

Citation 9

Author(s): Hertel, IV; Radloff, W

Title: Ultrafast dynamics in isolated molecules and molecular clusters

Source: REPORTS ON PROGRESS IN PHYSICS, 69 (6): 1897-2003 JUN 2006

Citation 10

Author(s): Vaupel, S; Brutschy, B; Tarakeshwar, P; Kim, KS

Title: Characterization of weak NH-π intermolecular interactions of ammonia with various substituted π-systems

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 128 (16): 5416-5426 APR 26 2006

Citation 11

Author(s): Tongraar, A; Kerdcharoen, T; Hannongbua, S

Title: Simulations of liquid ammonia based on the combined quantum mechanical/molecular mechanical (QM/MM) approach

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 110 (14): 4924-4929 APR 13 2006

Citation 12

Author(s): Perrine, CL; Zeller, M; Woolcock, J; Hunter, AD

Title: Crystal structure of ferrocenyl amine

Source: JOURNAL OF CHEMICAL CRYSTALLOGRAPHY, 35 (9): 717-721 SEP 2005

Citation 13

Author(s): Micek-Ilnicka, A; Gil, B; Lalik, E

Title: Ammonia sorption by Dawson acid studied by IR spectroscopy and microbalance

Source: JOURNAL OF MOLECULAR STRUCTURE, 740 (1-3): 25-29 APR 25 2005

Record 15

Author(s): Beu, TA; Buck, U

Title: Vibrational spectra of ammonia clusters from n=3 to 18

Source: JOURNAL OF CHEMICAL PHYSICS, 114 (18): 7853-7858 MAY 8 2001

Times Cited: 19

IF: 3.147

Punctaj citări: 10 x 13 = 130

Citation 1

Author(s): Lubombo, C (Lubombo, C.); Curotto, E (Curotto, E.); Barral, PEJ (Barral, Paula E. Janeiro); Mella, M (Mella, Massimo)

Title: Thermodynamic properties of ammonia clusters (NH₃)_n n=2-11: Comparing classical and quantum simulation results for hydrogen bonded species

Source: JOURNAL OF CHEMICAL PHYSICS, 131 (3): Art. No. 034312 JUL 21 2009

Citation 2

Author(s): Sigurbjornsson, OF (Sigurbjoernsson, Omar F.); Firanescu, G (Firanescu, George); Signorell, R (Signorell, Ruth)

Title: Intrinsic Particle Properties from Vibrational Spectra of Aerosols

Source: ANNUAL REVIEW OF PHYSICAL CHEMISTRY, 60: 127-146 2009

Citation 3

Author(s): Vrcek, V (Vrcek, Valerije); Mestric, H (Mestric, Hrvoje)

Title: Chlorination of ammonia and aliphatic amines by Cl₂: DFT study of medium and substituent effects

Source: JOURNAL OF PHYSICAL ORGANIC CHEMISTRY, 22 (1): 59-68 JAN 2009

Citation 4

Author(s): Pratihari, S (Pratihari, Subha); Chandra, A (Chandra, Amalendu)

Title: Microscopic solvation of a lithium atom in water-ammonia mixed clusters: Solvent coordination and electron localization in presence of a counterion

Source: JOURNAL OF CHEMICAL PHYSICS, 129 (2): Art. No. 024511 JUL 14 2008

Citation 5

Author(s): Salter, TE (Salter, Tom E.); Mikhailov, V (Mikhailov, Victor); Ellis, AM (Ellis, Andrew M.)

Title: Infrared photodissociation spectroscopy of Na(NH₃)_n clusters: Probing the solvent coordination

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (34): 8344-8351 AUG 30 2007

Citation 6

Author(s): Slipchenko, MN (Slipchenko, Mikhail N.); Sartakov, BG (Sartakov, Boris G.); Vilesov, AF (Vilesov, Andrey F.); Xantheas, SS (Xantheas, Sotiris S.)

Title: Study of NH stretching vibrations in small ammonia clusters by infrared spectroscopy in he droplets and ab initio Calculations

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (31): 7460-7471 AUG 9 2007

Citation 7

Author(s): Hu, YJ (Hu, Y. J.); Fu, HB (Fu, H. B.); Bernstein, ER (Bernstein, E. R.)

Title: Infrared plus vacuum ultraviolet spectroscopy of neutral and ionic ethanol monomers and clusters

Source: JOURNAL OF CHEMICAL PHYSICS, 125 (15): Art. No. 154305 OCT 21 2006

Citation 8

Author(s): Firanescu, G (Firanescu, George); Luckhaus, D (Luckhaus, David); Signorell, R (Signorell, Ruth)

Title: Size effects in the infrared spectra of NH₃ ice nanoparticles studied by a combined molecular dynamics and vibrational exciton approach

Source: JOURNAL OF CHEMICAL PHYSICS, 125 (14): Art. No. 144501 OCT 14 2006

Citation 9

Author(s): Firanescu, G (Firanescu, George); Hermsdorf, D (Hermsdorf, Dana); Ueberschaer, R (Ueberschaer, Roman); Signorell, R (Signorell, Ruth)

Title: Large molecular aggregates: from atmospheric aerosols to drug nanoparticles

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 8 (36): 4149-4165 2006

Citation 10

Author(s): Hertel, IV; Radloff, W

Title: Ultrafast dynamics in isolated molecules and molecular clusters

Source: REPORTS ON PROGRESS IN PHYSICS, 69 (6): 1897-2003 JUN 2006

Citation 11

Author(s): Vaupel, S; Brutschy, B; Tarakeshwar, P; Kim, KS
Title: Characterization of weak NH- π intermolecular interactions of ammonia with various substituted π -systems
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 128 (16): 5416-5426 APR 26 2006

Citation 12

Author(s): Micek-Ilnicka, A; Gil, B; Lalik, E
Title: Ammonia sorption by Dawson acid studied by IR spectroscopy and microbalance
Source: JOURNAL OF MOLECULAR STRUCTURE, 740 (1-3): 25-29 APR 25 2005

Citation 13

Author(s): Matsuda, Y; Mori, M; Hachiya, M; Fujii, A; Mikami, N
Title: Infrared spectroscopy of size-selected neutral clusters combined with vacuum-ultraviolet-photoionization mass spectrometry
Source: CHEMICAL PHYSICS LETTERS, 422 (4-6): 378-381 MAY 10 2006

Record 16

Author(s): Beu, TA; Onoe, J; Takeuchi, K
Title: Simulation of Raman spectra of C-60 and C-70 by non-orthogonal tight-binding molecular dynamics
Source: EUROPEAN PHYSICAL JOURNAL D, 10 (3): 391-398 JUN 2000
Times Cited: 10

IF: 1.421
Punctaj citări: 10 x 1 = 10

Citation 1

Author(s): Pokropivny, V (Pokropivny, V.); Kovrygin, S (Kovrygin, S.); Gubanov, V (Gubanov, V.); Lohmus, R (Lohmus, R.); Lohmus, A (Lohmus, A.); Vesi, U (Vesi, U.)
Title: Ab-initio calculation of Raman spectra of single-walled BN nanotubes
Source: PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, 40 (7): 2339-2342 MAY 2008

Record 17

Author(s): Beu, TA; Buck, U
Title: Evidence for chiral isomers in the spectra of small size selected hydrazine clusters
Source: ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-INTERNATIONAL JOURNAL OF RESEARCH IN PHYSICAL CHEMISTRY & CHEMICAL PHYSICS, 214: 437-447 Part 4 2000
Times Cited: 11

IF: 0.914
Punctaj citări: 10 x 7 = 70

Citation 1

Author(s): Zehnacker, A (Zehnacker, Anne); Suhm, MA (Suhm, Martin A.)
Title: Chirality recognition between neutral molecules in the gas phase
Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 47 (37): 6970-6992 2008

Citation 2

Author(s): Scharge, T (Scharge, Tina); Cezard, C (Cezard, Christine); Zielke, P (Zielke, Philipp); Schutz, A (Schuetz, Anne); Emmeluth, C (Emmeluth, Corinna); Suhm, MA (Suhm, Martin A.)
Title: A peptide co-solvent under scrutiny: self-aggregation of 2,2,2-trifluoroethanol
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 9 (32): 4472-4490 AUG 28 2007

Citation 3

Author(s): Picazo, O (Picazo, Oscar); Alkorta, I (Alkorta, Ibon); Elguero, J (Elguero, Jose); Sundberg, MR (Sundberg, Markku R.); Valo, J (Valo, Jaana)
Title: Bonding properties related with chiral discrimination in dinuclear metal complexes of group 10
Source: EUROPEAN JOURNAL OF INORGANIC CHEMISTRY, (2): 324-332 JAN 2007

Citation 4

Author(s): Alkorta, I (Alkorta, Ibon); Zborowski, K (Zborowski, Krzysztof); Elguero, J (Elguero, Jose)
Title: Self-aggregation as a source of chiral discrimination
Source: CHEMICAL PHYSICS LETTERS, 427 (4-6): 289-294 AUG 31 2006

Citation 5

Author(s): Alkorta, I; Picazo, O; Elguero, J
Title: Chiral recognition in self-complexes of tetrahydroimidazo[4,5-d]imidazole derivatives: From dimers to heptamers
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 110 (6): 2259-2268 FEB 16 2006

Citation 6

Author(s): Picazo, O; Alkorta, I; Elguero, J
Title: Dimers of 1,8a-dihydro-1,8-naphthyridine derivatives as models of chiral self-recognition
Source: STRUCTURAL CHEMISTRY, 16 (3): 339-345 JUN 2005

Citation 7

Author(s): Alkorta, I; Picazo, O; Elguero, J
Title: Chiral recognition in cyclic alpha-hydroxy carbonyl compounds: A theoretical study
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 109 (14): 3262-3266 APR 14 2005

Record 19

Author(s): Siebers, JG; Buck, U; Beu, TA
Title: Calculation of structures and vibrational spectra of acetonitrile clusters
Source: CHEMICAL PHYSICS, 239 (1-3): 549-560 DEC 15 1998
Times Cited: 17

IF: 1.707
Punctaj citări: 10 x 6 = 60

Citation 1

Author(s): Nigam, S (Nigam, Sandeep); Majumder, C (Majumder, Chiranjib)
Title: Growth pattern and electronic properties of acetonitrile clusters: A density functional study
Source: JOURNAL OF CHEMICAL PHYSICS, 128 (21): Art. No. 214307 JUN 7 2008

Citation 2

Author(s): Mennucci, B (Mennucci, Benedetta); da Silva, CO (da Silva, Clarissa O.)
Title: A quantum mechanical strategy to investigate the structure of liquids: The cases of acetonitrile, formamide, and their mixture
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 112 (22): 6803-6813 JUN 5 2008

Citation 3

Author(s): Timerghazin, QK (Timerghazin, Qadir K.); Peslherbe, GH (Peslherbe, Gilles H.)
Title: Electronic structure of the acetonitrile and acetonitrile dimer anions: A topological investigation
Source: JOURNAL OF PHYSICAL CHEMISTRY B, 112 (2): 520-528 JAN 17 2008

Citation 4

Author(s): Alia, JM (Alia, Jose M.); Edwards, HGM (Edwards, Howell G. M.); Fawcett, WR (Fawcett, W. Ronald); Smagala, TG (Smagala, Thomas G.)
Title: An experimental Raman and theoretical DFT study on the self-association of acrylonitrile
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 111 (5): 793-804 FEB 8 2007

Citation 5

Author(s): Schweke, D; Haas, Y; Dick, B
Title: Photophysics of phenylpyrrole derivatives and their acetonitrile clusters in the gas phase and in argon matrixes: Simulations of structure and reactivity
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 109 (17): 3830-3842 MAY 5 2005

Citation 6

Author(s): Schweke, D; Baumgarten, H; Haas, Y; Rettig, W; Dick, B
Title: Charge-transfer-type fluorescence of 4-(1H-pyrrol-1-yl)benzonitrile (PBN) and N-phenylpyrrole (PP) in cryogenic matrixes: Evidence for direct excitation of the CT band
Source: JOURNAL OF PHYSICAL CHEMISTRY A, 109 (4): 576-585 FEB 3 2005

Record 22

Author(s): Beu, TA; Buck, U; Siebers, JG; Wheatley, RJ
Title: A new intermolecular potential for hydrazine clusters: Structures and spectra
Source: JOURNAL OF CHEMICAL PHYSICS, 106 (17): 6795-6805 MAY 1 1997
Times Cited: 15

IF: 3.247
Punctaj citări: 10 x 2 = 20

Citation 1

Author(s): Dyczmons, V (Dyczmons, Volker)
Title: Structures and vibrations of the dimers and trimers of hydrazine/water
Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 766 (1): 9-13 JUN 30 2006

Citation 2

Author(s): Du, DM; Fu, AP; Zhou, ZY
Title: Theoretical study of chiral discrimination in the hydrogen bonding complexes of the hydrazine dimer
Source: INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, 101 (3): 340-347 JAN 20 2005

Record 23

Author(s): Beu, TA; Buck, U; Ettischer, I; Hobein, M; Siebers, JG; Wheatley, RJ

Title: Vibrational predissociation spectra of size selected hydrazine clusters: Experiment and calculations

Source: JOURNAL OF CHEMICAL PHYSICS, 106 (17): 6806-6812 MAY 1 1997

Times Cited: 16

IF: 3.247

Punctaj citări: 10 x 2 = 20

Citation 1

Author(s): Dyczmons, V (Dyczmons, Volker)

Title: Structures and vibrations of the dimers and trimers of hydrazine/water

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, 766 (1): 9-13 JUN 30 2006

Citation 2

Author(s): Du, DM; Fu, AP; Zhou, ZY

Title: Theoretical study of chiral discrimination in the hydrogen bonding complexes of the hydrazine dimer

Source: INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, 101 (3): 340-347 JAN 20 2005

Record 24

Author(s): Beu, TA; Onoe, J; Takeuchi, K

Title: Calculations of structure and IR-spectrum for small UF₆ clusters

Source: JOURNAL OF CHEMICAL PHYSICS, 106 (14): 5910-5919 APR 8 1997

Times Cited: 12

IF: 3.247

Punctaj citări: 10 x 1 = 10

Citation 1

Author(s): Eerkens, JW

Title: Laser-induced migration and isotope separation of epi-thermal monomers and dimers in supercooled free jets

Source: LASER AND PARTICLE BEAMS, 23 (2): 225-253 JUN 2005

Record 25

Author(s): BEU, TA; TAKEUCHI, K

Title: STRUCTURE AND IR-SPECTRUM CALCULATIONS FOR SMALL SF₆ CLUSTERS

Source: JOURNAL OF CHEMICAL PHYSICS, 103 (15): 6394-6413 OCT 15 1995

Times Cited: 28

IF: 3.610

Punctaj citări: 10 x 7 = 70

Citation 1

Author(s): Tokhadze, IK (Tokhadze, Irina K.); Kolomiitsova, TD (Kolomiitsova, Tatjana D.); Shchepkin, DN (Shchepkin, Dmitrii N.); Tokhadze, KG (Tokhadze, Konstantin G.); Mielke, Z (Mielke, Zofia)

Title: Influence of Resonance Interactions and Matrix Environment on the Spectra of SF₆ Dimers in Low-Temperature Nitrogen Matrixes. Theory and Experiment

Source: JOURNAL OF PHYSICAL CHEMISTRY A, 113 (22): 6334-6341 JUN 4 2009

Citation 2

Author(s): Olivet, A (Olivet, Aurelio); Vega, LF (Vega, Lourdes F.)

Title: Optimized molecular force field for sulfur hexafluoride simulations

Source: JOURNAL OF CHEMICAL PHYSICS, 126 (14): Art. No. 144502 APR 14 2007

Citation 3

Author(s): Tokhadze, IK (Tokhadze, I. K.); Kolomiitsova, TD (Kolomiitsova, T. D.); Tokhadze, KG (Tokhadze, K. G.); Shchepkin, DN (Shchepkin, D. N.)

Title: The effect of resonance interactions on the absorption spectra of (SF₆)₂ dimers in low-temperature matrices: Calculations and experiment

Source: OPTICS AND SPECTROSCOPY, 102 (3): 396-407 MAR 2007

Citation 4

Author(s): Ignatov, SK; Kolomiitsova, TD; Mielke, Z; Razuvaev, AG; Shchepkin, DN; Tokhadze, KG

Title: A matrix isolation and theoretical study of SiF₄ dimers spectra

Source: CHEMICAL PHYSICS, 324 (2-3): 753-766 MAY 31 2006

Citation 5

Author(s): Boychenko, IV; Huber, H

Title: Beyond the resonant dipole interaction model: Resolution of a discrepancy between experimental and calculated structures of the carbon dioxide cyclic planar trimer

Source: JOURNAL OF CHEMICAL PHYSICS, 124 (1): Art. No. 014305 JAN 7 2006

Citation 6

Author(s): Olivet, A; Duque, D; Vega, LF

Title: Sulfur hexafluoride's liquid-vapor coexistence curve, interfacial properties, and diffusion coefficients as predicted by a simple rigid model

Source: JOURNAL OF CHEMICAL PHYSICS, 123 (19): Art. No. 194508 NOV 15 2005

Citation 7

Author(s): Eerkens, JW

Title: Laser-induced migration and isotope separation of epi-thermal monomers and dimers in supercooled free jets

Source: LASER AND PARTICLE BEAMS, 23 (2): 225-253 JUN 2005

Record 26

Author(s): BEU, TA

Title: PERTURBATION APPROACH FOR FREQUENCY-SHIFTS IN IR-SPECTRA OF MOLECULAR CLUSTERS

Source: ZEITSCHRIFT FUR PHYSIK D-ATOMS MOLECULES AND CLUSTERS, 31 (1-2): 95-104 AUG 1994

Times Cited: 14

IF: 1.512

Punctaj citări: 10 x 1 = 10

Citation 1

Author(s): Boychenko, IV; Huber, H

Title: Beyond the resonant dipole interaction model: Resolution of a discrepancy between experimental and calculated structures of the carbon dioxide cyclic planar trimer

Source: JOURNAL OF CHEMICAL PHYSICS, 124 (1): Art. No. 014305 JAN 7 2006

Record 28

Author(s): BEU, TA; MERCEA, PV

Title: GAS-TRANSPORT THROUGH METALLIZED POLYMER MEMBRANES

Source: MATERIALS CHEMISTRY AND PHYSICS, 26 (3-4): 309-322 NOV 1990

Times Cited: 16

IF: 0.561

Punctaj citări: 10 x 4 = 40

Citation 1

Author(s): Fahlteich, J (Fahlteich, John); Fahland, M (Fahland, Matthias); Schonberger, W (Schoenberger, Waldemar); Schiller, N (Schiller, Nicolas)

Title: Permeation barrier properties of thin oxide films on flexible polymer substrates

Source: THIN SOLID FILMS, 517 (10): 3075-3080 MAR 31 2009

Citation 2

Author(s): Jang, C (Jang, Changsoo); Cho, YR (Cho, Young-Rae); Han, B (Han, Bongtae)

Title: Ideal laminate theory for water transport analysis of metal-coated polymer films

Source: APPLIED PHYSICS LETTERS, 93 (13): Art. No. 133307 SEP 29 2008

Citation 3

Author(s): Greener, J (Greener, J.); Ng, KC (Ng, K. C.); Vaeth, KM (Vaeth, K. M.); Smith, TM (Smith, T. M.)

Title: Moisture permeability through multilayered barrier films as applied to flexible OLED display

Source: JOURNAL OF APPLIED POLYMER SCIENCE, 106 (5): 3534-3542 DEC 5 2007

Citation 4

Author(s): Davis, LM (Davis, Luke M.); Thompson, DS (Thompson, D. Scott); Dean, CJ (Dean, C. J.); Pevzner, M (Pevzner, M.); Scott, JL (Scott, J. L.); Broadwater, ST (Broadwater, S. T.); Thompson, DW (Thompson, D. W.); Southward, RE (Southward, R. E.)

Title: Silver-polyimide nanocomposite membranes: Macromolecular-matrix-mediated metallization of an aromatic, fluorinated polyimide yielding highly reflective films at low metal concentrations

Source: JOURNAL OF APPLIED POLYMER SCIENCE, 103 (4): 2409-2418 FEB 15 2007

Record 30

Author(s): BEU, TA; SPINEANU, F; VLAD, M; CAMPEANU, RI; POPESCU, II

Title: TOPIC - A TOKAMAK PLASMA IMPURITIES CODE

Source: COMPUTER PHYSICS COMMUNICATIONS, 36 (2): 161-176 1985

Times Cited: 5

IF: 1.598

Punctaj citări: 10 x 4 = 40

Citation 1

Author(s): Maddaluno, G (Maddaluno, G.); Zagorski, R (Zagorski, R.); Ridolfini, VP (Ridolfini, V. Pericoli); Apicella, ML (Apicella, M. L.); Calabro, G (Calabro, G.); Crisanti, F (Crisanti, F.); Cucchiaro, A (Cucchiaro, A.); Pizzuto, A (Pizzuto, A.); Ramogida, G (Ramogida, G.)

Title: Edge plasma physics issues for the Fusion Advanced Studies Torus (FAST) in reactor relevant conditions

Source: NUCLEAR FUSION, 49 (9): Art. No. 095011 SEP 2009

Citation 2

Author(s): Zhou, Q (Zhou Qian); Wu, ZW (Wu Zhenwei); Huang, J (Huang Juan)

Title: The spectroscopic systems for the study of light impurity particle transport in the HT-7 tokamak

Source: PLASMA SCIENCE & TECHNOLOGY, 9 (1): 23-29 FEB 2007

ISSN: 1009-0630

Citation 3

Author(s): Zhang, XM (Zhang Xian-Mei); Wan, BN (Wan Bao-Nian); Wu, ZW (Wu Zhen-Wei)

Title: Estimation of charge exchange recombination emission based on diagnostic neutral beam on the experimental advanced superconducting Tokamak

Source: CHINESE PHYSICS LETTERS, 24 (2): 487-489 FEB 2007

Citation 4

Author(s): Zhou, Q; Wan, BN; Wu, ZW; Huang, J

Title: The carbon impurity particle transport in ohmic discharges on the HT-7 tokamak

Source: CHINESE PHYSICS, 14 (12): 2539-2545 DEC 2005

Record 32

Author(s): BEU, TA; CAMPEANU, RI

Title: PROLATE RADIAL SPHEROIDAL WAVE-FUNCTIONS

Source: COMPUTER PHYSICS COMMUNICATIONS, 30 (2): 177-185 1983

Times Cited: 11

IF: 1.598

Punctaj citări: 10 x 4 = 40

Citation 1

Author(s): Kirby, R (Kirby, R.)

Title: Calculation of radial prolate spheroidal wave functions of the second kind

Source: COMPUTER PHYSICS COMMUNICATIONS, 181 (3): 514-519 MAR 2010

Citation 2

Author(s): Deng, SZ (Deng, Shaozhong)

Title: Electrostatic potential of point charges inside dielectric oblate spheroids

Source: JOURNAL OF ELECTROSTATICS, 67 (5): 807-814 SEP 2009

Citation 3

Author(s): Deng, S (Deng, Shaozhong)

Title: Electrostatic potential of point charges inside dielectric prolate spheroids

Source: JOURNAL OF ELECTROSTATICS, 66 (11-12): 549-560 NOV 2008

Citation 4

Author(s): Kirby, P (Kirby, P.)

Title: Calculation of spheroidal wave functions

Source: COMPUTER PHYSICS COMMUNICATIONS, 175 (7): 465-472 OCT 1 2006

Record 34

Author(s): CAMPEANU, RI; BEU, T

Title: HYDROGEN ANTIHYDROGEN INTERACTION POTENTIAL

Source: PHYSICS LETTERS A, 93 (5): 223-226 1983

Times Cited: 13

IF: 2.142

Punctaj citări: 10 x 2 = 20

Citation 1

Author(s): Armour, EAG; Richard, JM; Varga, K

Title: Stability of few-charge systems in quantum mechanics

Citation 2

Author(s): Van Hooydonk, G

Title: The 4-particle hydrogen-antihydrogen system revisited - Twofold molecular Hamiltonian symmetry and natural atom antihydrogen

Source: EUROPEAN PHYSICAL JOURNAL D, 32 (3): 299-317 MAR 2005

4. Distincții, premii și alte recunoașteri naționale și internaționale

Se acorda 10 puncte pentru fiecare distincție, premiu

Formula de calcul: 10 puncte x nr. distincții, premii

5. Studenți naționali (activități de coordonare științifică și didactică) 49

Îndrumare lucrari de licență și disertație (număr lucrări susținute):

Formula de calcul:

3 puncte x [(număr de proiecte, lucrări de licență) / număr de conducători științifici]

4 puncte x [(număr de lucrări de masterat conduse) / număr de conducători științifici]

Doctoranzi (lista nominală a doctoranzilor înmatriculați resp. lista nominală a tezelor susținute)

Formula de calcul:

6 puncte x nr. doctoranzi înmatriculați

10 puncte x nr. teze susținute

15 puncte x nr. teze co-tutela susținute

Post-doctoranzi (lista nominală)

Formula de calcul:

8 puncte x nr. post-doctoranzi

Licență – 15

- Horváth Lóránd
- Gînscă Otilia Daniela
- Florescu Ana-Maria
- Ghișoiu Ioan
- Cabău Gabriel

Masterat – 8

- Horváth Lóránd
- Florescu Ana-Maria

Doctoranzi înmatriculați – 18

- Horváth Lóránd
- Kiss Attila
- Pop Sergiu

Post-doctoranzi – 8

- Jurjiu Aurel

6. Studenți internaționali atrași (activități de coordonare științifică și didactică)

- Îndrumare lucrari de licență (număr lucrări susținute):

- Îndrumare lucrări de disertație (număr lucrări susținute):

Formula de calcul:

6 puncte x [(număr de proiecte, lucrări de licență) / număr de conducători științifici]

8 puncte x [(număr de lucrări de masterat conduse) / număr de conducători științifici]

- Doctoranzi (lista nominală a doctoranzilor înmatriculați resp. lista nominală a tezelor susținute)

Formula de calcul:

12 puncte x nr. doctoranzi înmatriculați

20 puncte x nr. teze susținute

- Post-doctoranzi (lista nominală)

Formula de calcul:
16 puncte x nr. post-doctoranzi

7. Membru in comitetul de redacție la reviste ISI

Formula de calcul:
10 puncte x nr. comitete

8. Membru in comitetul de redacție la reviste BDI

Formula de calcul:
5 puncte x nr. comitete

9. Participări la programe/granturi de cercetare finanțate din sursă internațională (se menționează și valoarea)

Formula de calcul: valoarea in RON / 8.000

10. Participări la programe/granturi finanțate din sursă națională (se menționează și valoarea)

287.7

Formula de calcul: valoarea in RON / 10.000

1. "Procese de transport si structurare la scara micro/nanometrica in biomedicina si stiinta materialelor", CEEX – NANOSIM / 2005
Valoare: 100000 lei
Punctaj: 100
2. "Studiul rețelelor de doturi cuantice și a nanostructurilor de carbon", PN-II ID 502 / 2007
Valoare: 976950 lei
Punctaj: 97.69
3. "Modelarea nanostructurilor carbonului si a derivatilor lor functionalizati", PN-II ID 506 / 2007
Valoare: 900000 lei
Punctaj: 90

11. Coordonări de programe/granturi finanțate din sursă internațională (se menționează și valoarea)

Formula de calcul: valoarea intrata in UBB in RON / 8.000

12. Coordonări de programe/granturi finanțate din sursă națională (se menționează și valoarea)

202.7

Formula de calcul: valoarea intrata in UBB in RON / 5.000

1. "Calculare de proprietati structurale si dinamice pentru clusteri, nanostructuri si nanodispozitive de interes tehnologic si biologic", CNCSIS 1310 / 2006
Valoare: 900000 lei
Punctaj: 180
2. "Simulări computaționale și studii teoretice privind filme amorfe și nanostructuri de carbon și seleniu" – COOPBIL – Ungaria RO-28/2007, RO ID 13
Valoare: 113345.26 lei
Punctaj: 22.66

13. Profesor invitat la universitati de prestigiu, cu titlu oficial

Formula de calcul: 20 puncte x invitatii

14. Membru în comisii profesionale relevante, cu titlu oficial

240

Formula de calcul: 5 puncte x nr. invitatii

Membru în Consiliul Național al Cercetării Științifice din Invățământul Superior (CNCSIS), Comisia de Matematică și Științe ale Naturii.

15. Conferințe invitate internaționale

Se acorda 20 puncte pentru fiecare Conferința și se ține cont de numărul de autori.

Formula de calcul: $20 / \text{număr de autori}$

16. Membru în comitete de organizare sau științifice ale unor conferințe internaționale

20

Se acorda 20 puncte pentru fiecare comitet.

Formula de calcul: $20 \times \text{nr. comitete}$

Membru în comitetul de organizare al Conferinței internaționale "4th Conference on Elementary Processes in Atomic Systems, Cluj-Napoca, Romania, June 18-20, 2008"

Criteriul III – Realizare remarcabilă – pondere 10%

(Descrieți într-o manieră cât mai accesibilă (în maximum 1 pagină) cea mai importantă realizare științifică/tehnică/artistică din ultimii 5 ani și impactul acesteia.).

NANOSIM – Laborator pentru simularea sistemelor nanostructurate

A fost realizat un laborator de cercetare în fizică computațională, cu o echipare la standarde internaționale. Au fost utilizate exclusiv fondurile proiectelor de cercetare atrase de subsemnat. Puterea de calcul implică 200 de procesoare de ultimă generație. A fost realizată o bibliotecă de aplicații performante de dinamică moleculară și calcule ab initio. Au fost atrași doctoranzi și a fost repatriat un post-doctorand.

$$\text{Total punctaj} = 0,6 \times 2573,0 + 0,3 \times 2009,4 = \mathbf{2146,6}$$

Data: 15.03.2010

Semnătura:

Certific validitatea datelor prezentate

Sef de catedră,