

Publication list

Written by Administrator

Wednesday, 05 June 2013 08:50 - Last Updated Wednesday, 31 January 2018 22:42

2018

25. S. N. Fejer, R. G. Mantell, D. J. Wales; Mol. Phys. (in press)

Designing Hierarchical Molecular Complexity: Icosahedra of Addressable Icosahedra

2017

24. Z. Antal, J. Szoverfi and S. N. Fejer, J. Chem. Inf. Model, 57(4), 910-917 (2017).

Predicting the Initial Steps of Salt Stable Cowpea Chlorotic Mottle Virus Capsid Assembly with Atomistic Force Fields

2015

23. S. N. Fejer and D. J. Wales, Soft Matter 11(33), 6663-6668 (2015).

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Design of a Kagome lattice from soft anisotropic particles

2014

22. S. N. Fejer, D. Chakrabarti, H. Kusumaatmaja and D. J. Wales, *Nanoscale* 6(16), 9448-9456 (2014).

Design principles for Bernal spirals and helices with tunable pitch

21. B. Jójárt, M. Posa, B. Viskolcz and S. N. Fejer, *J. Chem. Phys.* 140(14), 144302 (2014).

Global optimization of cholic acid aggregates

2013

20. S. W. Olesen, S. N. Fejer, D. Chakrabarti and D. J. Wales, *RSC Advances* 3, 12905-12908 (2013)

A left-handed building block self-assembles into right- and left-handed helices

19. C. J. Forman, S. N. Fejer, D. Chakrabarti, P. Barker and D. J. Wales, *J. Phys. Chem. B*, 117, 7918-7928 (2013)

Local frustration determines molecular and macroscopic helix structures (also featured on the cover of the journal)

18. I. Jákli, I. G. Csizmadia, S. N. Fejer, Ö. Farkas, B. Viskolcz, S. J. Knak Jensen, A. Perczel, *Chem. Phys. Lett.*, 563, 80-87 (2013).

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Helix compactness and stability: Electron structure calculations of conformer dependent thermodynamic functions

2011

17. S. N. Fejer, D. Chakrabarti and D. J. Wales, *Soft Matter*, 7, 3553-3564 (2011).

Self-assembly of anisotropic particles

16. D. Chakrabarti, S. N. Fejer and D. J. Wales, Royal Society of Chemistry Theoretical and Computational Book Series 4: Computational Nanoscience (2011).

Self-assembly of nanoclusters: An energy landscape perspective

2010

15. S. N. Fejer, D. Chakrabarti and D. J. Wales, *ACS Nano*, 4, 219-228 (2010).

Emergent complexity from simple anisotropic building blocks: Shells, tubes and spirals

14. M.S. Bauer, B. Strodel, S.N. Fejer, E.F. Koslover and D.J. Wales, *J. Chem. Phys.*, 132, 054101 (2010).

Interpolation Schemes for Peptide Rearrangements

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13. E. Malolepsza, B. Strodel, M. Khalili, S. A. Trygubenko, S. N. Fejer and David J. Wales, J. Comp. Chem., 131, 1402-1409 (2010).

Symmetrisation of the AMBER and CHARMM Force Fields

2009

12. D. Chakrabarti, S. N. Fejer and D. J. Wales, Proc. Natl. Acad. Sci. USA, 106, 20164-20167 (2009).

Rational design of helical architectures

11. S. N. Fejer, T. R. James, J. Hernández-Rojas and D. J. Wales, Phys. Chem. Chem. Phys. 11, 2098–2104 (2009).

Energy landscapes for shells assembled from pentagonal and hexagonal pyramids

2007

10. B. Viskolcz, M. Szori, R. Izsak, S. N. Fejer and I. G. Csizmadia, Int. J. Quant. Chem. 107, 1826–1834 (2007).

Thermodynamic functions of conformational changes, Part IV: Functional analysis of conformational entropy of substituted ethane and methanol

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9. S. N. Fejer and D. J. Wales, *Phys. Rev. Lett.* 99 (8), 086106 (2007).

Helix self-assembly from anisotropic molecules

8. B. Viskolcz, S. N. Fejer, S. J. K. Jensen, A. Perczel and I. G. Csizmadia, *Chem. Phys. Lett.* 40, 123–126 (2007).

Information accumulation in helical oligopeptide structures

2006

7. B. Viskolcz, S. N. Fejer, M. Szori and I. G. Csizmadia, *Mol. Phys.* 104,795–803 (2006).

Thermodynamic functions of conformational changes I. A comparative first principle study on 1,2-disubstituted ethanes

6. B. Viskolcz, S. N. Fejer and I. G. Csizmadia, *J. Phys. Chem. A* 110, 3808–3813 (2006).

Thermodynamic functions of conformational changes II: conformational entropy as a measure of information accumulation

5. M. A. Sahai, S. N. Fejer, B. Viskolcz, E. F. Pai, and I. G. Csizmadia, *J. Phys. Chem. A* 110, 11527–11536 (2006).

First-principle computational study on the full conformational space of L-threonine diamide, the energetic stability of cis and trans isomers

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4. S. N. Fejer, B. Viskolcz and I. G. Csizmadia, J. Phys. Chem. A 110, 13325–13331 (2006).

Thermodynamic functions of conformational changes III: Conformational network of glycine diamide folding, entropy lowering and information accumulation

2005

3. J. M. S. Law, S. N. Fejer, D. H. Setiadi, G. A. Chass and B. Viskolcz, J. Mol. Struct. (THEOCHEM) 722, 79–96 (2005).

Molecular orbital computations on lipids. An ab initio exploratory study on the conformations of glycerol and its fluorine congeners

2. C. M. Nagy, S. N. Fejer, L. Berek, J. Molnar and B. Viskolcz, J. Mol. Struct. (THEOCHEM) 726, 55-59 (2005).

Hydrogen bondings in deoxynivalenol (DON) conformations

2004

1. S. N. Fejer, Z. A. Jenei, G. Paragi, J. Mol. Struct. (THEOCHEM) 666-667, 303-310 (2004)

Conformational effects of the valine sidechain on the betaLbetaL extended and type I beta turn backbone structures of MECO-Val-Ala-NHMe and MeCO-Ala-Val-NHMe