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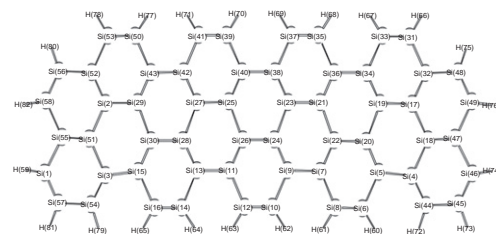
REGULAR PAPERS

1–4

On the possibility of zigzag and armchair silicon nanoribbons having the graphene structure

Michael Miller and Frank J. Owens

Density functional molecular calculations of the minimum energy structure of armchair nanoribbons show that they have the same two dimensional structure as graphene and are stable as free standing structures. However, the planar zigzag structure is shown to not be a minimum energy structure having negative vibrational frequencies. The armchair ribbons have small direct band gaps which decrease with ribbon length approaching metallic behavior. The difference in the density of states between the spin up state and down state at the top of the valence level raises the possibility that the ribbons could be ferromagnetic semiconductors.

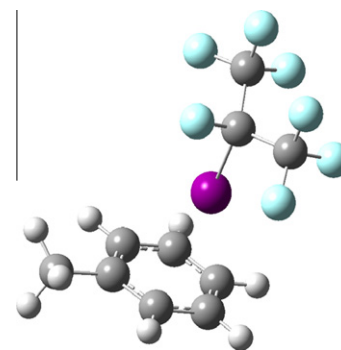


5–10

A ^{19}F NMR study of $\text{C}-\text{I} \cdots \pi$ halogen bonding

D. Hauchecorne, B.J. van der Veken, W.A. Herrebout and P.E. Hansen

^{19}F NMR spectra of solutions of the perfluoroiodopropanes $1-\text{C}_3\text{F}_7\text{I}$ and $2-\text{C}_3\text{F}_7\text{I}$ with toluene- d_8 reveal the formation of van der Waals complexes, with strengths varying between -2.7 and -2.9 kJ mol^{-1} .

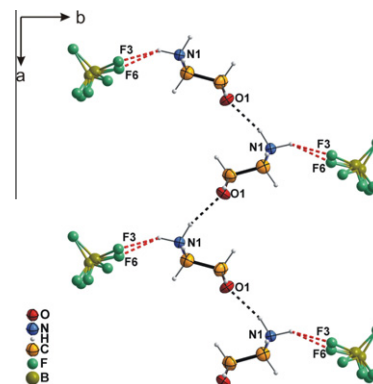


11–20

Vibrational and thermodynamic properties and molecular motions in the incommensurate crystal of morpholinium tetrafluoroborate studied by ^1H NMR

M. Owczarek, R. Jakubas, G. Bator, A. Pawlukojć, J. Baran, J. Przesławski and W. Medycki

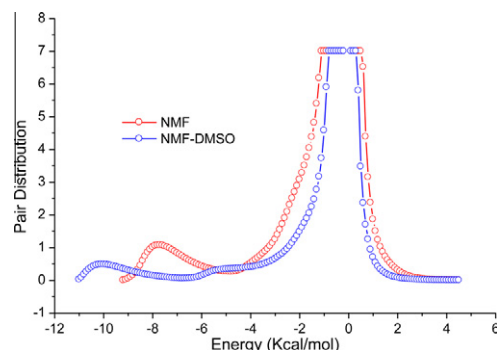
The $\text{N}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{F}$ hydrogen bond system determines the dynamical properties and the phase transitions sequence in $[\text{NH}_2(\text{C}_2\text{H}_4)_2\text{O}][\text{BF}_4]$.



21–28**Investigation on the structure of liquid *N*-methylformamide–dimethylsulfoxide mixtures**

João M.M. Cordeiro and Alan K. Soper

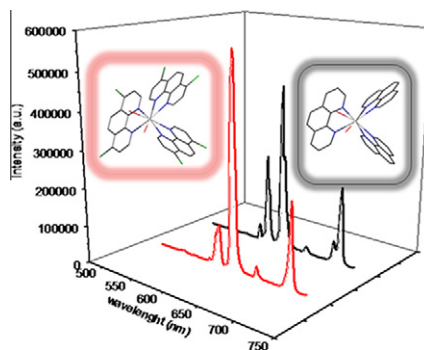
Structure of liquid NMF and DMSO mixtures investigated using a combination of neutron diffraction techniques augmented with isotopic substitution and empirical potential structure refinement simulations.



29–34**Eu(III) complex luminescence behavior upon chlorine substitution in the 1,10-phenanthroline ligand: A theoretical and experimental study**

Mônica F. Belian, Hécio J. Batista, Ana Gabriela S. Bezerra, Wagner E. Silva, Gilberto F. de Sá and Severino Alves Jr.

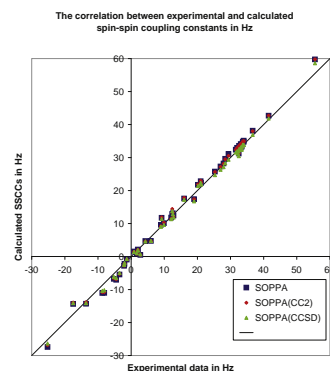
In this work, it were performed computational design and synthesis of a new luminescent Eu(III) complex with the usual 1,10-phenanthroline ligand substituted in the 4 and 7 positions by chlorine atoms, which one has shown a higher luminescent output than that of the non-substituted analogous complex.



35–43**Benchmarking SOPPA(CC2) for the calculation of indirect nuclear spin–spin coupling constants: Carbocycles**

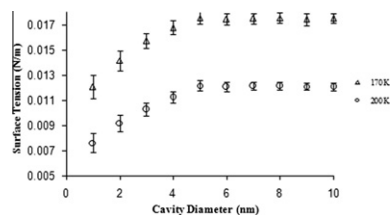
Hanna Kjær, Stephan P.A. Sauer, Jacob Kongsted, Yury Yu. Rusakov and Leonid B. Krivdin

The performance of the SOPPA(CC2) method for the calculation of indirect nuclear carbon–carbon spin–spin coupling constants is tested on 197 coupling constants in 41 carbocycles.



44–48**Size dependence and effect of potential parameters on properties of nano-cavities in liquid xenon using molecular dynamics simulation**

Hamed Akbarzadeh, Hadi Abroshan, Farid Taherkhani, Cobra IZanloo and Gholam Abbas Parsafar



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