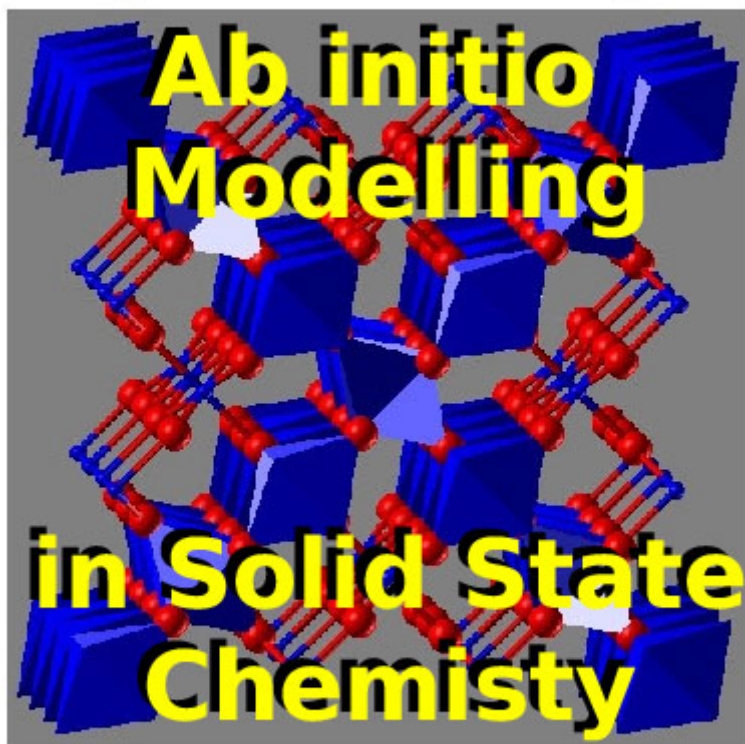


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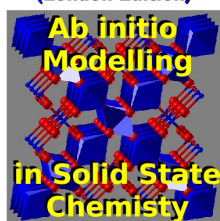


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POSTERS

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DANIEL DRUMM

University of Melbourne

**Density Functional Theory Modelling of
Delta-Doped Phosphorus in Silicon**

Density Functional Theory models of 0.25 monolayer phosphorus in silicon using various functionals were constructed and contrasted. Measures of efficacy included the amount of surrounding silicon "cladding" required to converge several properties to stable values, and direct comparison of these values to experimental data.

HIROYUKI FUENO

Kyoto University

The Electronic Structures of Conjugated Polymers with Acetylenyl Bridges

*Hiroyuki Fueno, Takuya Saeki and Kazuyoshi Tanaka
Department of Molecular Engineering, Graduate School of Engineering,
Kyoto University, Katsura Nishikyo-ku, Kyoto 615-8510, Japan*

The low dimensional carbon materials such as carbon nanotube or graphene sheet have attracted much attention as electronic materials.

In this study, we dealt with the graphyne sheet, which is two-dimensional conjugated carbon material involving phenylacetylene unit (Fig. 1). Then, it has triple bonds in the polymer unit. We analyzed the band structures and the crystal orbital patterns of graphyne by the CRYSTAL06 program.

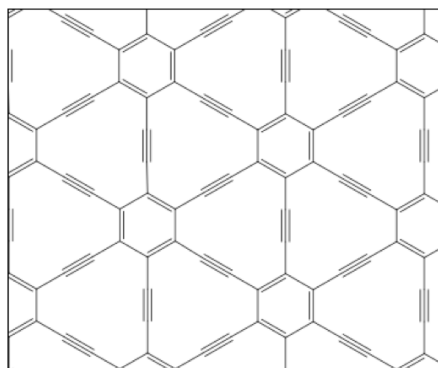


Fig. 1 The graphyne sheet.

It has been theoretically found that the well-known carbon-carbon bond alternations and band gaps in the simple-conjugated organic polymers tend to reduce in their heavily-doped regime, that is, the 'counter Peierls transition' [1].

The structures of graphyne were optimized in the neutral and the cationic (hole injection) states. The results indicate the 'counter Peierls' distortion as shown in Fig. 2.

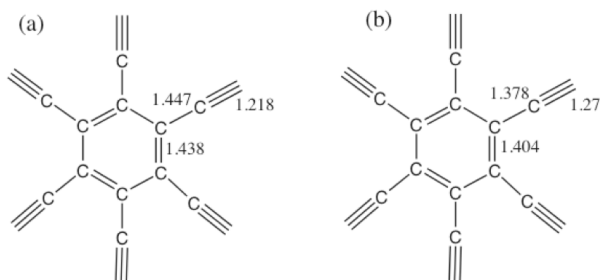
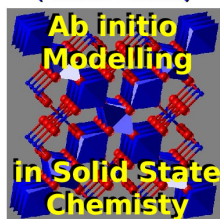


Fig. 2 The optimized structures of unit cell in (a) the neutral and (b) the 6 holes states by the B3LYP/STO-6G.

References

[1] K. Tanaka, M. Okada, T. Koike, T. Yamabe, *Synthetic Metals*, 31, 181 (1989).

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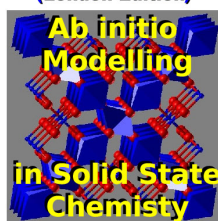
JOSE LUIS MENDOZA-CORTES

California Institute of Technology

Outstanding Methane Uptake in Covalent Organic Frameworks: Theory and Experiment

We report methane uptake at 298 K and pressure (1 to 100 bar) in a variety of covalent organic frameworks (COFs). For all systems, we predicted the uptake using grand canonical Monte Carlo (GCMC) simulations using quantum mechanics based force fields (FF), which we validate with experimental results. The FF parameters were developed from the second order Møller-Plesset perturbation theory calculations using doubly-polarized quadruple (QZVPP) basis sets for various CH₄-CH₄, CH₄-C₆H₆, CH₄-B₃O₃H₃, and CH₄-Si(CH₄)₄ configurations. This FF was validated with the equation of state for CH₄. Experimental uptake isotherms at 298 K are reported for COF-5 and COF-8, which agree well with the GCMC simulations. We predict that one of our materials can store a total of 195 v/v of CH₄, exceeding the US Department of Energy target for CH₄ storage of 180 v/v at 298K and 35 bar. We also report uptakes in a delivery amount basis, where at 100 bar COF-102 and COF-103 have an uptake of 230 and 234 v(STP)/v, respectively, showing that these are promising materials for practical methane storage.

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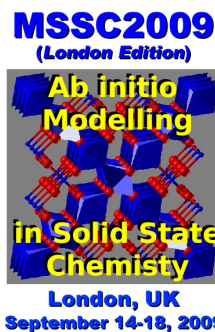
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YANARIS ORTEGA GARCIA

University of Seville

A Density Functional Theory Study of Gold Atoms Supported on Anatase Modified with Nitrogen

The interaction between nitrogen impurities, gold adsorption and oxygen vacancies at the anatase TiO₂ (101) surface is investigated by periodic density functional theory calculations. Substitutional and interstitial configurations for the N impurities have been considered, as well as, several adsorption sites for the Au adatom and different types of vacancies. Our total energy calculations suggest that nitrogen doping favors the adsorption of gold and vacancy formation. It is predicted that the creation of vacancies on the anatase modified with nitrogen and gold atoms supported produce migration of N substitutional impurities from bulk to surface sites. In general, the most stable configurations are those where N, Au and the vacancies are in close proximity. The electronic structure reveals that the presence of vacancies modifies the oxidation state of N and Au, presenting an electron transfer that is quantified by the Bader charges. The gap is slightly reduced by the N-doping, and discrete levels appear in the middle of the gap. It is shown how the gold adatom and vacancies modify the gap and the occupation of midgap states. Hence, the optical and photocatalytic properties are modified.



WEIYE QIAO

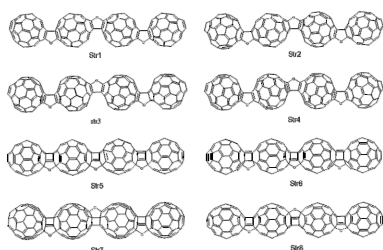
Beijing Normal University

Crystal Orbital Studies on One-dimensional C₆₀O Polymers and Its Combination Structures with Carbon Nanotubes

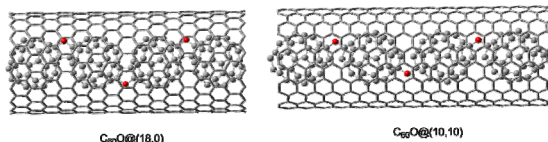
*Weiye Qiao¹ Xinqian Li¹ Yuanhe Huang*¹*

¹ College of chemistry, Beijing Normal University, Beijing 100875, China

It has been found that the covalent C₆₀O polymeric chains can be formed from C₆₀O reacting inside carbon nanotubes (CNT) [1]. For the understanding of structure-property relationship of this polymers, the structures and electronic properties of one-dimensional (1D) C₆₀O polymers are investigated using DFT-PBE methods with Gaussian 03 and Crystal 06 program packages. Eight 1D models of C₆₀O are constructed and optimized. The self-consistent crystal calculations show that the stability of 1D C₆₀O polymers are mainly determined by the positions and strain of the carbon atoms forming the inter cage bonds between the neighbor C₆₀ cages. The neutral polymers are all semiconductors. The rigid-band theory is valid for the corresponding anionic polymers. Several combination structures made of 1D C₆₀O chains inserted inside carbon nanotubes (C₆₀O@CNT) are also explored. Covalent bonds are formed between the C₆₀ cages and the carbon nanotube wall in C₆₀O@(12,0). It is found that the distance between the C₆₀O chain and the carbon nanotube wall is close to 3.4 Å for the most stable peapod studied from a view of energy. Followings are the obtained structures for the C₆₀O polymers and the two combination systems.



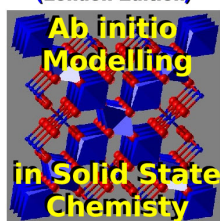
Models of the one-dimensional C₆₀O polymers



Structures of C₆₀O@(18,0) and C₆₀O@(10,10)

[1]David A.Britz,Andrei N.Khlobystov,et.al.Chem.Commun.,2005, 37.

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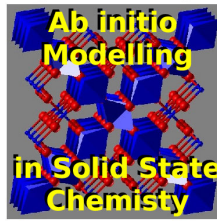
AISHA SYEDA RAHMAN

University College London

High Pressure Study of the C₂N₃H System with a Defect Wurtzite Structure

Theoretical and experimental results are presented for the C₂N₃H system formed at high temperature and high pressure. The proton ordering is also investigated to see if the positioning of the H affects the overall stability of the structure. The C₂N₃H system is confirmed to have a defect wurtzite structure, XRD patterns and Raman Spectra are presented.

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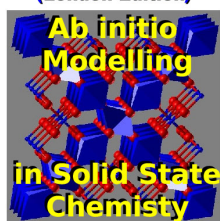
VICENTE TIMÓN SALINERO

University College London

DFT Theoretical Study about the Iron Isomorphous Substitution in Biotites Micas

Under the scheme of DFT with the use of SIESTA code we study the influence of the Iron substitution in the electrical behaviour and structure of thriooctahedral biotite micas.

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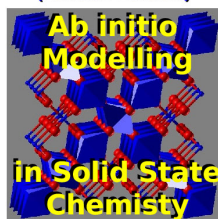
PAOLO SERENI

University of Salzburg

Measurement of the Raman Tensor of Stibnite (Sb₂S₃)

Since sulfide minerals are potentially attractive materials for thermoelectric and photovoltaic applications, our group is performing a research programme aimed at measuring the Raman tensor of Stibnite, Sb₂S₃, a naturally occurring sulfosalt semiconducting mineral with a band gap of approximately 1.4-1.74 eV. X-ray diffraction pole figure technique was used to determine the structural properties of the single crystalline sample. Polarization-dependent Raman spectroscopic measurements have been performed for various sample orientations using both a visible and an infrared laser excitation line (532 and 1064 nm, respectively). The polarization-dependent analysis yields 10 A_g, 5 B_{1g}, 10 B_{2g} and 5 B_{3g} Raman active modes from the five non-equivalent sites. The corresponding phonon frequencies have been calculated using the PHONON/WIEN2k codes. The obtained measurement results are here presented and compared with the values predicted by the calculations.

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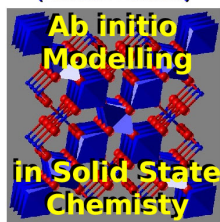
DARREN SIMPSON

University of South Australia

The Effect of Iron and Copper Dopants on Sphalerite Flotation Behaviour

The outcome from this study has provided new information concerning the effect of impurities in sphalerite (zinc sulfide) on flotation behaviour. These findings suggest a reason why previous articles have reported conflicting results on sphalerite flotation. Surface energies calculated from the semi-empirical SCFMO method MSINDO indicate that a sphalerite 110 surface containing Fe is more hydrophilic than a pure zinc sulfide surface while the surface containing Cu is more hydrophobic. The latter is in agreement with the literature and supports the use of Cu activation in sphalerite flotation. Outcomes from calculations on surface models with adsorbed non-polar species also highlight the connection between Fe content and the potential for carbon-based contamination.

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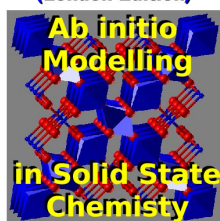
MARIA SORIANO SANTACRUZ

University of Alicante

Computational Studies of Magnetic and Electronic Properties of Metal-Phthalocyanines on Surfaces

A group of 3d-transition metal-phthalocyanines adsorbed on copper, silver and gold surfaces, have been studied with the quantum-chemistry Gaussian code. As a first step, the gas-phase electronic structure of the molecules and the isolated metals has been computed in order to understand and forecast changes in electronic and magnetic properties of the molecules after deposition. The metal-molecule system has finally been computed and the charge transfer and concomitant lose or gain of magnetic moment has been investigated.

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VIMAL VYAS

Banasthali University

Compton Profile Study of Some Semiconductor Compounds

In this paper we report on the Compton Profile study of some semiconductor compounds like ZnSe, CdTe, AlN and BN etc. using 59.54 keV gamma-rays.