

allows us to determine the relevance of several structural parameters in the process of complexation, thus adding to the rational building of more efficient ligands. The initial state of the simulations is taken from X-ray diffraction results<sup>[1]</sup> which are also used to verify that the simulations predictions are in agreement with experimental data.

[1] de Namor A.F.D., Chahine S., Kowalska D., Castellano E.E., Piro O.E., *J. Am. Chem. Soc.*, 2002, **124**, 12824-12836.

**Keywords:** molecular dynamics, calixarene complexes, small molecules

#### P.03.04.3

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#### Structural Properties of Pt-based Anti-cancer Drugs; Computational Studies

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It is generally accepted that *cis*-[PtCl<sub>2</sub>Pyr<sub>2</sub>] is cytotoxic while *trans*-[PtCl<sub>2</sub>Pyr<sub>2</sub>] is not. Although original empirical structural-activity studies indicated *trans* Pt complexes as being inactive as anti-cancer drugs, it has subsequently been found that *trans*-[PtCl<sub>2</sub>Pyr<sub>2</sub>] is in fact active, both *in vitro* and *in vivo*, and that for the latter the compound is even more active than the corresponding *cis* form. A more likely explanation for the lack of antitumour activity is instead that the *trans* isomer is kinetically more reactive and more susceptible to deactivation than the corresponding *cis* form [1].

We have in the current work investigated both isomers and their corresponding step-wise activation (aquation) processes in order to provide more detailed insights into their mechanisms. The results are also compared to corresponding data for the parent compounds *cis* and *trans*-platin [PtCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub>]. Implicit as well as explicit solvent effects have previously been shown to be important for these types of reactions [2,3], and thus included in the study.

[1] Wong E., Giandomenico M., *Chem. Rev.*, 1999, **99**, 2451. [2] Raber J., Zhu C., Eriksson L.A., *Mol. Phys.*, 2004, **102**, 2537. [3] Zhu C., Raber J., Eriksson L.A., *J. Phys. Chem. B*, 2005, *in press*.

**Keywords:** anticancer compounds, DFT, platinum antitumour agents

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#### Effect of Nanoscale Surface Modification on Interfacial Adhesion: a Theoretical Modelling Study

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The effects of modification of polyester surfaces on adhesion to carbonaceous solids are investigated using theoretical techniques. Fully atomistic models are constructed of cross-linked polyester and glassy carbon surfaces. Polyester surface modifiers of both the hydrophilic and hydrophobic nature are introduced and simulations are then performed to obtain qualitative and quantitative measures of interfacial strength between the polyester and carbon thin layers [1].

Our studies indicate that Van der Waals forces contribute significantly to the interfacial strength between the thin layers while atomic scale surface roughness is found to significantly reduce adhesion. Interfaces formed from rigid surface models provide general information on structural and chemical effects but such rigid models tend to overestimate the magnitude of these effects. Relaxed interfacial models provide more realistic representations on interactions between the layers. Flexible chain-based modifiers on the surface of the polyester films tend to migrate away from the interface and flatten the surface thereby decreasing the roughness effects on interfacial strength. Both hydrophilic and hydrophobic surface modifications resulted in reduced adhesion at the interface.

[1] Henry D. J., Lukey C. A., Evans E., Yarovsky I., *Mol. Sim.*, *in press*.

**Keywords:** adhesion, surface modification, molecular modelling

#### P.03.05.2

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#### Modeling of Crystal Structures of Materials: Which Goals can be Achieved?

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Ability to predict structures of crystalline materials is important in many cases for practical applications. For instance, second harmonic generation by crystalline nonlinear optical materials necessarily require acentric structure of their crystals. Crystal structure is also important for high-energy materials, where molecular packing defines crystal density. Some other properties such as fluorescence, conductivity and even potency of drugs are also related to their crystal structure.

We analyzed effectiveness of different force fields for crystal structure prediction for group of organic nonlinear optical, high-energy and conductive materials. It was shown that for non-planar molecules improvement of a force field could bring to a significant improvement of results. On the other hand crystal structure of planar molecules is difficult to predict, and in this case some new approaches for instance implementation of "stacking forces" should be introduced.

**Keywords:** crystal structure modeling, force fields, crystalline materials

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#### A Global Search for the Optimal Bandstructure for Thermoelectric Applications

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The best thermoelectric (TE) materials over the last 30 years has been Bi<sub>2</sub>Te<sub>3</sub> and its alloys. However recent discoveries have renewed the interest in finding a better TE material. We've decided to use a global search genetic algorithm to try and determine the optimal bandstructure for materials with TE applications. This project involves bandstructure analysis and transport property calculations of known materials with interesting TE properties. We want to employ a genetic algorithm to try and locate general features in a bandstructure which have importance for the TE effect of the material.

**Keywords:** density functional theory, band structure, transport properties

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#### Computer Modeling of Local Structure and Properties of Oxide Solid Solutions with NaCl Type Structure

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Atomistic semi-empirical potentials were applied to calculate the structural, thermodynamic, elastic properties and phase equilibrium of MgO-CaO, MgO-MnO, MnO-CaO, CaO-SrO, BaO-SrO disordered solid solutions by using of the GULP code [1]. The calculations were performed with partially covalent approximations for 7:1, 3:1, 1:1, 1:3, 1:7 randomly mixed cation compositions. It was used 256-ion primitive supercell with quadrupled parameters of the unit cell for all compositions. It was demonstrated that such supercell allows to imitate random distribution of cations.

On the basis of the calculated values of free energy the component fields of stability, mixing limits and critical temperature were predicted. The values are in a good agreement within the temperature range 298 – 1800 K with the available data and results of other theoretical investigation. For 1:1 composition the analyses of the local