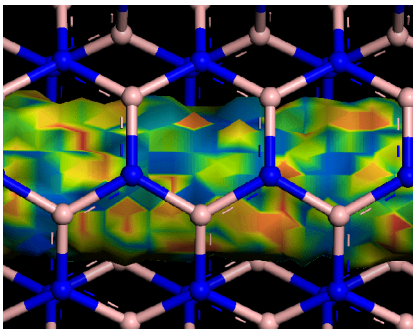
CASE STUDY

A NEW SOLVATION MODEL FOR POLYMERS AND SURFACES – ACCURATE PREDICTION OF THE THERMODYNAMIC PROPERTIES OF MIXTURES



Predicting the solvated behavior of materials is a critical step in materials innovation

"The DMol3-COSMO method is modified and generalized to work for periodic boundary conditions. "

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Industry sectors

- Chemicals
- Petrochemicals
- Pharmaceuticals

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Reporting in the journal Molecular Simulation, Bernard Delley from the Paul Scherrer Institute in Villigen, Switzerland, has revisited and generalized the DMol^3-COSMO method[1] for describing solvation effects for polymers and surfaces within periodic boundary conditions.[2]

The new solvation model which employs continuous solvent accessible surfaces also works for solid materials with internal surfaces and proves useful for calculations such as geometry optimizations, molecular dynamics, and vibrational analysis. The methods devised can be used to accurately predict the thermodynamic properties of mixtures.

INTRODUCTION

The Conductor-like Screening Model (COSMO) is a well established method to introduce solvation effects into quantum chemical calculations.[3] Its original implementation in Accelrys' DMol^3 program had the drawback that it only worked for molecular systems and was not applicable to periodic systems such as surfaces or bulk phases. In this work the DMol^3-COSMO method is modified and generalized to work for periodic boundary conditions. In this way solvation effects can now also be calculated for polymers, surfaces, and internal surfaces in solids.

RESULTS

In order to extend the existing DMol^3-COSMO model the scientists introduced a new way of calculating the solvent accessible surface (SAS).[2] This grid used for setting up the SAS is now a continuous function of all atomic geometries. This property is desirable for all calculations

in which molecular geometry changes such as geometry optimization, molecular dynamics or vibrational analysis.

Tests on a set of 290 molecules showed the same standard deviation of 0.36 kcal/mol for COSMOtherm predictions as with the previous model.[3,4] These predictions included calculation of thermodynamic properties such as free energy of hydration, vapor pressures, and partition coefficients. The new model proved also consistent with the older parameterization when free solvation enthalpies of glycine and polythiophene polymers were calculated.[2]

The generalization of the DMol^3-COSMO model to surfaces such as the α-Quartz surface displayed in Fig. 1 may open a new era in modeling liquid-solid interfaces. Now the chemistry at the interface between the liquid and the solid state can be studied by keeping only a few of the solvent molecules – as needed – and modeling the rest of them with the COSMO model.

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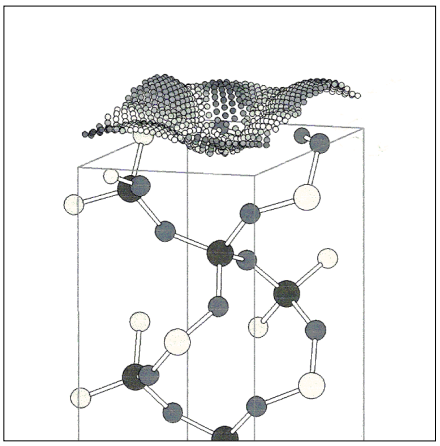

Figure 1. *COSMO charges for a hydroxylated α-Quartz (0001) surface. Silicon atoms are displayed as dark balls, oxygen atoms as light color balls.*

REFERENCES

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4. A. Klamt and V. Jonas, J. Chem. Phys., 1**05, 9972 (1996)**.