Chemistry Central Journal

Oral presentation

Crystal structures of moderately complex organic molecules are predictable

J Van de Streek* and MA Neumann

Address: Avant-garde Materials Simulation Deutschland GmbH, Merzhauserstr. 177, 79100 Freiburg im Breisgau, Germany
* Corresponding author

from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):O13 doi:10.1186/1752-153X-3-S1-O13

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/O13

A comprehensive computational strategy for the prediction of crystal structures is presented that has scored an unprecedented 4 in 4 success rate at the 2007 international Crystal-Structure Prediction Blind Test [1]. Key components of the new approach, implemented in the GRACEsoftware package, are a dispersion-corrected Density Functional Theory (DFT) method developed in-house for the accurate calculation of lattice energies [2], a robust procedure for the parameterisation of non-transferable force fields on a per molecule basis [2], and a novel approach for crystal-structure generation. The dispersion-corrected DFT method combines DFT calculations by means of the VASPprogram with an empirical Van der Waals correction; it is used for the final lattice energy ranking and acts as a reference standard for force-field parameterisation. A tailor-made force field is derived for each molecule to be considered and used for crystal-structure generation as well as for the preparation of second derivative matrices for the final lattice-energy optimisations with the dispersion-corrected DFT method. Based on the known statistical deviation between the tailor-made force field and the dispersion-corrected DFT method, it is possible to select a shortlist of crystal structures from a small energy window for the final lattice-energy optimisations and ranking of the predicted crystal structures with the dispersion-corrected DFT method. In addition to the Blind Test results, validation studies for 15 organic molecules are presented, including ethane, ethylene, acetylene, methanol, urea, acetic acid, cyclohexane-1,4-dione, paracetamol, previous Blind Test molecules I to VI and a pharmaceutical compound for which crystal structures have been predicted in a blind test fashion. 17 out of the 18 experimentally observed crystal forms of these molecules are found among the first two most stable predicted crystal structures.

References

1. Neumann MA, Leusen FJJ, Kendrick J: *Angew Chem Int Ed* 2008, **47:**2427-2430.
2. Neumann MA, Perrin M-A: *J Phys Chem B* 2005, **109:**15531-15541.
3. Neumann MA: *J Phys Chem* 2008 in press.