Poster Presentation

IT.P14

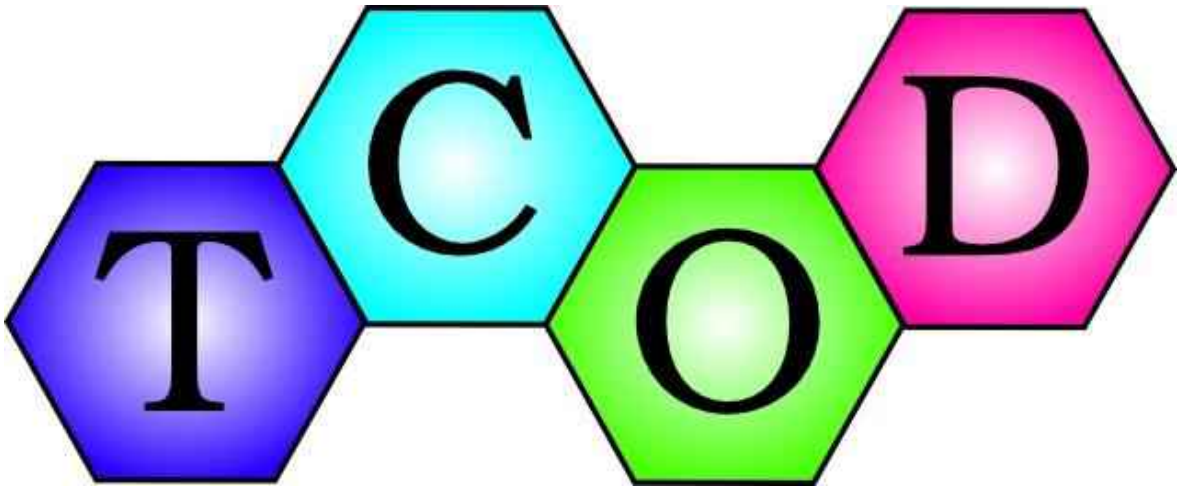
Launching the Theoretical Crystallography Open Database

S. Gražulis[1], A. Merkys[1], A. Vaitkus[2], A. Le Bail[3], D. Chateigner[4,5,6], L. Vilčiauskas[7], S. Cottenier[8], T. Björkman[9], P. Murray-Rust[10]

[1]Vilnius University Institute of Biotechnology, Department of Protein - DNA Interactions, Vilnius, Lithuania, [2]Vilnius University Faculty of Mathematics and Informatics, Department of Mathematical Computer Science, Vilnius, Lithuania, [3]Université du Maine, Laboratoire des Oxydes et Fluorures, Le Mans, France, [4]Université de Caen-Basse Normandie, UMR 6508 CRISMAT, Caen, France, [5]ENSICAEN, UMR 6508 CRISMAT, Caen, France, [6]CNRS, UMR 6508 CRISMAT, Caen, France, [7]Department of Chemistry, New York University, New York, USA, [8]Ghent University, Center for Molecular Modeling (CMM) & Department of Materials Science and Engineering (DMSE), Zwijnaarde, Belgium, [9]Aalto University School of Science, COMP/Department of Applied Physics, Espoo, Finland, [10]The University of Cambridge, Department of Chemistry, Cambridge, UK

As computational chemistry methods enjoy unprecedented growth, computer power increases and price/performance ratio drops, a large number of crystal structures can today be refined and their properties computed using modern theoretical approaches, such as DFT, post-HF, QM/MM, MCMM methods. Availability of several open source codes for computational and quantum chemistry and open-access crystallographic databases enables large scale computations of material structures and properties. We thus increasingly feel that an open collection of theoretically computed chemical structures would be a valuable resource for the scientific community. To address this need, we have launched a Theoretical Crystallography Open Database (TCOD, http://www.crystallography.net/tcod/). The TCOD sets a goal to collect a comprehensive set of computed crystal structures that would be made available under an Open Data license and invites all scientists to deposit their published results or pre-publication data. Accompanied with a large set of experimental structures in the COD database [1], the TCOD opens immediate possibilities for experimental and theoretical data cross-validation. To ensure high quality of deposited data, TCOD offers ontologies in a form of CIF [2] dictionaries that describe parameters of computed chemical and crystal structures, and an automated pipeline that checks each submitted structure against a set of community-specified criteria for convergence, computation quality and reproducibility. The scope of TCOD and validation tools make TCOD a high-quality, comprehensive theoretical structure database, useful in a broad range of disciplines. First-principle calculations are also of huge interest to simulate physical properties, either prospectively or for materials that do not grow as sufficiently large crystals. The property results can now be tested against the Material Properties Open Database [3] (http://www.materialproperties.org/) to ameliorate the used models.

[1] *Gražulis S., Daškevič A., Merkys A., et al., Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration Nucleic Acids Research, 2012, 40, D420-D427,* ***[2]*** *Hall, S. R.; Allen, F. H. & Brown, I. D. The crystallographic information file (CIF): a new standard archive file for crystallography Acta Crystallographica Section A, 1991, 47, 655-685,* ***[3]*** *Pepponi, G.; Gražulis, S. & Chateigner, D. MPOD: A Material Property Open Database linked to structural information Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms , 2012, 284, 10 - 14*



Keywords: Crystallographic databases, Chemical databases, Computational chemistry