## MS38-P18 Integration of theoretical crystallography open database and AiiDA

Andrius Merkys[1,2], Giovanni Pizzi[1], Andrea Cepellotti[1], Nicolas Mounet[1], Saulius Gražulis[2], Nicola Marzari[1]

1. Theory and Simulation of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland
2. Vilnius University Institute of Biotechnology, Graičiūno 8, LT-02241 Vilnius, Lithuania

email: andrius.merkys@gmail.com

Over almost a quarter of century of existence, Crystallographic Information Framework (CIF) format – an unified format for reporting and storage of the results of experimental crystal structure solutions – has been widely adopted and used as a de facto standard by most of crystallographic journals as well as structural databases (Inorganic Crystal Structure Database, Crystallography Open Database (COD, http://www.crystallography.net)). New CIF dictionaries are being developed with the aim of unambiguously defining ontologies in order to homogenize the data in various fields of crystallography. However, much effort is still needed to be put in for the field of theoretical crystallography, which is expanding quickly thanks to the unprecedented developments of electronic structure methods, the increase of computer power and the decrease of the price/performance ratio. The Theoretical Crystallography Open Database (TCOD, http://www.crystallography.net/tcod/) has been launched in order to collect the results of calculations, performed by the plethora of theoretical calculation groups using various modern theoretical approaches (DFT, post-HF,QM/MM, etc.), into an open-access resource. TCOD, together with the large set of experimental structures in the COD, opens the possibility for experimental-theoretical data cross-validation. TCOD has adopted the best practice of using the CIF format, approach-specific dictionaries and defining data validation criteria for automated checks. Furthermore, TCOD puts an emphasis on the provenance and reproducibility of the results by devising a special dictionary for related metadata. Recently, this dictionary was used as an interface for the integration of the TCOD with the AiiDA framework (http://www.aiida.net), a high-throughput infrastructure that provides a high-level research environment to automate the execution of computations, automatically store inputs and results in a tailored database (with particular care in always keeping track of the full provenance of all data) and share the results. Such an integration of calculation automation frameworks and database storage allows for deposition of simulation results with automatically recorded metadata, guaranteeing the reproducibility of each calculation as well as the full data provenance for each item in the database. Moreover, data from the TCOD database can be easily retrieved and imported back into the AiiDA framework as an input for further calculations and analyses.

**Keywords:** theoretical crystallography, structural databases, research environment software

## MS38-P19 Structural characterization of complex LDH samples and TGA-GC-MS study of thermal response and carbonate contamination in nitrate and organic-exchanged hydrotalcites

Marco Milanesio[1], Eleonora Conterosito[1], Luca Palin[1], Valentina Gianotti[1], Luana Perioli[2], Enrico Mugnaioli[3], Ute Kolb[4], Davide Viterbo[1], Diego Antonioli[1]

1. Dipartimento di Scienze e Innovazione Tecnologica, Università del Piemonte Orientale "A. Avogadro" Via Michel 11, I-15121 Alessandria, Italy
2. Dipartimento di Scienze Farmaceutiche Università degli Studi di Perugia Via del Liceo 1, I-06123 Perugia, Italy
3. Dipartimento di Scienze Fisiche, della Terra e dell'Ambiente, Università degli Studi di Siena Via Laterino 8, 53100 Siena, Italy
4. Institut für Physikalische Chemie, Johannes Gutenberg Universität, Jakob-Welder-Weg 11, 55099 Mainz, Germany

email: marco.milanesio@unipmn.it

Layered double hydroxides (LDH) are versatile materials used for intercalating bioactive molecules, both in pharmaceutical, nutraceutical and cosmetic fields, with the purpose of protecting them from degradation, enhancing their water solubility to increase bioavailability, to improve pharmacokinetics properties and formulation stability. The crystal chemistry of hydrotalcite-like compounds is investigated by X-ray powder diffraction (XRPD), automated electron diffraction tomography (ADT) and hyphenated TGA-GC-MS to shed light on the mechanisms involved in ion exchange and absorption of contaminants, mainly carbonate anions. For the first time ADT allowed to obtain a structural model of LDH_$NO_3$ from experiment, shedding light on the conformation of nitrate inside LDH and on the loss of crystallinity due to the layer morphology. The ADT analysis of a hybrid LDH sample (LDH_EUS) clearly revealed the increase of defectivity in this material. XRPD demonstrated that the presence of carbonate is able to drive the intercalation of organic molecules into LDH, since $CO_3$ contaminated samples tend to assume d-spacings roughly multiples of LDH_$CO_3$ d-spacing. TGA-GC-MS allowed distinguishing and quantifying intercalated and surface adsorbed organic molecules, confirming the presence and amount of carbonate, especially at low (below 2% in weight) concentrations and separating the different types and strength of adsorption, in relation with the temperature of elimination.

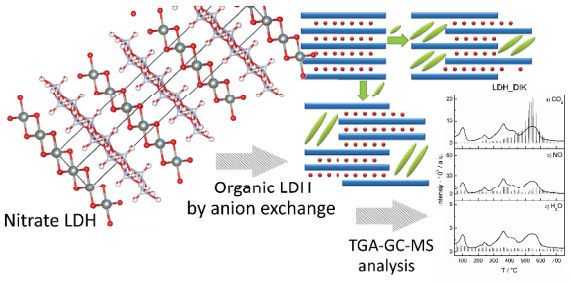


**Figure 1.** A model for ion exchange in hydrotalcite by combining XRPD, ED/ADT and TGA-GC-MS

**Keywords:** LDH thermal response, TGA-GC-MS, automated electron diffraction tomography, ionic exchange mechanism