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DiffPy-CMI - a software toolbox for real-space structure analysis and Complex Modeling

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This presentation and the associated hands-on tutorial will introduce DiffPy-CMI, a software for structure analysis from experimental atomic Pair Distribution Function (PDF) and for Complex Modeling [1, 2]. DiffPy-CMI (Complex Modeling Infrastructure) has been developed to handle ill-posed inverse problems, where diffraction experiments do not provide enough signal to determine complicated structures or nanostructures. To overcome this problem, we use a Complex Modeling approach [3] which allows users to combine additional experimental or theoretical inputs and uses them all together in a common optimization routine. DiffPy-CMI is a flexible and extensible program allowing user to create such models tailored for the specific knowledge about the material under study. DiffPy-CMI runs on Linux and Mac operating systems and is primarily written in Python with computationally intense parts coded in C++. It can also be run on windows using the Windows Linux Subsystem (WSL). In the big picture DiffPy-CMI provides several ways of representing atomic structures, a set of forward calculators (e.g., PDF, bond valence sums, powder and single crystal diffraction), and finally a fit-manager to define and run multi-input refinements. The fits can be conducted with short Python scripts or within the Jupyter Notebook interactive environment. In addition to Complex Modeling, DiffPy-CMI also enables more subtle PDF refinements which are not possible in PDFgui [4] - for example PDF fits of non-periodic small clusters or of molecular crystals with rigid structure units. The software provides access to internal simulation routines, which can be tweaked or extended, and thus permits rapid implementation of new ideas and more accurate models. We will demonstrate the capabilities of DiffPy-CMI on a series of science cases, starting from simple forward calculations and following up with PDF fitting examples that go beyond PDFgui.

[1] P. Juhás, et al., Acta Crystallogr. A 71 (2015), 562-568.

DiffPy-CMI is available at https://www.diffpy.org.

S. J. L. Billinge, I. Levin, Science 316 (2007), 561-565.

C. L. Farrow et al., J. Phys: Condens. Mat. 19 (2015), 335219.

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