Oral presentation

Uniting Aspherical Atom Models and NoMoRe refinement in AAM_NoMoRe approach: enhanced results and server applications

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Since its inception, X-ray diffraction (XRD) has become a pivotal method for material structure characterization. Advancements in theory, experimentation, and technology have led to remarkably accurate diffraction patterns. Extracting comprehensive information from these patterns requires models that account for both electron density and thermal motion. While electron density modelling has progressed significantly, thermal motion treatment has remained stagnant for a long time.

To address this, we developed AAM_NoMoRe, a method combining charge density models (like HAR [1, 2] or TAAM [3]) with the thermal motion model (NoMoRe [4]), refining frequencies from ab-initio calculations instead of routine atomic displacement parameters (ADPs). We demonstrated the efficacy of AAM_NoMoRe on compounds like alanine, xylitol, naphthalene, and glycine polymorphs, showcasing its impact on hydrogen atom positions and ADP shapes, akin to neutron data. The approach exhibited great fitting performance, with consistently lower wR2 values compared to IAM refinement and a significant decrease compared to traditional NoMoRe. On average, AAM_NoMoRe improved wR2 values by approximately 5% pp across all systems, comparable to HAR or TAAM models. Additionally, we successfully estimated the heat capacity, aligning well with experimental data.

To go further, we would like to demonstrate free of charge AAM_NoMoRe web server which enables for refinement of frequencies of normal modes evaluated using periodic DFT calculations against single crystal X-ray data and calculates ADPs based on data from HAR or TAAM refinement. Additionally, it allows to calculate thermodynamic parameters like vibrational entropy or heat capacity.

Jayatilaka, D., Dittrich, B. (2008). *Acta Cryst. A*., **64**, 383.

[1] Capelli, S. C., Burgi, H. -B., Dittrich, B., Grabowsky, S. & Jayatilaka, D. (2014). *IUCrJ*, **1**, 361.

[2] K. K. Jha, K. K., Gruza, B., Kumar, P., Chodkiewicz, M. L. & Dominiak, P. M. (2020). *Acta Cryst*, *A.,* **76**, 296.

[3] Hoser, A. A., Madsen, A. Ø. (2016). *Acta Cryst. A*, **72**, 206.

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