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Modeling molecular crystals with fragment-based electronic structure techniques

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A proper theoretical description of molecular crystal packing requires a uniformly high-quality treatment of the diverse intra- and intermolecular interactions. Fragment-based electronic structure methods enable the application of accurate electronic structure approaches to chemically interesting molecular crystals by decomposing the total crystal energy into the sum of many smaller "fragment" calculations. In this talk, we will discuss (1) the hybrid quantum/classical fragment based approach we have developed for molecular crystal problems, (2) state-of-the-art electronic structure approaches for treating the individual fragments with the requisite accuracy and acceptable computational effort, and (3) applications of these techniques to interesting molecular crystal problems.

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