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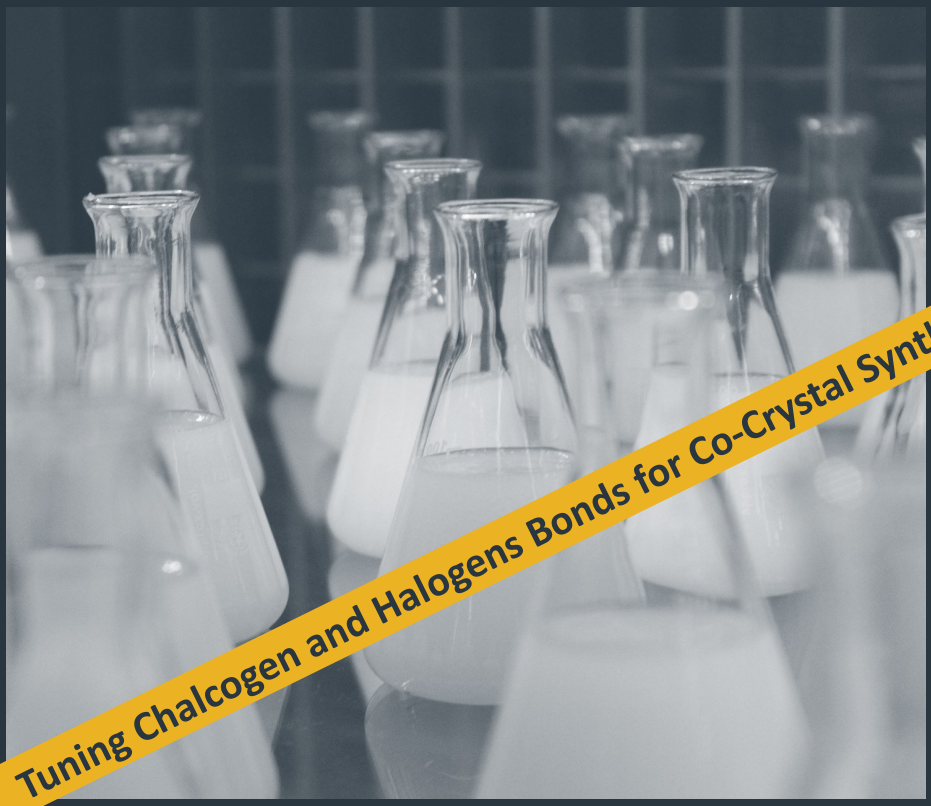

Tuning Chalcogen and Halogens Bonds for Co-Crystal Synthesis

Fine-tuning of intermolecular interactions in co-crystal engineering has shown great importance for the design of energetic materials and pharmaceuticals. In addition to the traditional hydrogen bonds, halogen, chalcogen and pnictogen bonds are gaining attention as tools to create more elaborate and diverse structural assemblies. In this work, computational chemistry calculations are used to predict the structure of molecular systems that can form both halogen and chalcogen bonds. An energy decomposition analysis is also performed to determine the nature of the intermolecular forces driving the formation of these non-covalent interactions. Functionalization strategies to increase the tunability of these intermolecular interactions are obtained. The results will contribute to the design of new crystalline materials.

Emilie Guidez

Assistant Professor, Department of Chemistry

University of Colorado Denver

Oct

30

Via Zoom

11am-12pm

UNIVERSITY OF COLORADO DENVER CHEMISTRY DEPARTMENT