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Structure-property correlation from quantum crystallography perspective

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Understanding the structure-property correlation in molecular materials is crucial for predicting the mechanical, electrical and optical properties of bulk materials. Our primary goal is to elucidate how molecules self-assemble in the crystalline state and to identify which intermolecular interactions determine specific physical properties. Among many possibilities, quantum crystallography (QCr) approach seems perfect for this task, as it combines experimental and theoretical methods to extract essential information. Using this methodology, we integrate high-resolution X-ray diffraction data with quantum chemical calculations to study intermolecular interactions in organic and organometallic crystalline materials.

In this work, we present a set of QCr tools that lead to accurate prediction of molecular and bulk properties. The presented workflow allows us to identify reproducible structural features that are transferable between different systems, which in turn leads to a better understanding of molecular self-assembly processes that promote specific crystal packing and thus prominent material properties.

Author: KRAWCZUK, Anna Malgorzata (Georg-August-Universitaet Gottingen (DE))

Presenter: KRAWCZUK, Anna Malgorzata (Georg-August-Universitaet Gottingen (DE))

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