Extended Molecular Representations for Electronic-Structure Informatics and Their Applications

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Molecules' electronic structures determine most of their properties and chemical reactivity. Therefore, molecular representations must be sophisticated enough to predict and interpret these characteristics using AI and machine learning methods. So far, we have suggested that electronic structure informatics (ESI), which handles information at the electronic structure level, would be helpful and promising in providing unique molecular representations for property predictions. In this talk, we will discuss the plausible extension of molecular representations under some principles in ESI and some applications along this line.