Electronic-Structure Informatics: Concepts, Extended Methods, and Recent Applications

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We have been suggesting “Electronic-Structure Informatics (ESI)” as one of the informatics methods for chemistry and materials science. It focuses on information related to the electronic structures of molecules and materials without directly referring to their structural characteristics. In the lecture, concepts of ESI will be introduced on the basis of quantum chemical theories of molecules and in solid-state physics. This informatics method seems advantageous for, in particular, scaffold hopping to find functional molecules and materials. Recent extensions and applications of the ESI descriptors for machine learning and *in silico* screening will also be discussed. They will include two discussions on the applicability of ESI: one is on natural-product-based drug discovery, and another is on the prediction of the regioselectivity of drug metabolites in e.g. glutathione conjugation.