Covalent and Non-Covalent Interactions in Molecular Systems

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This talk will concern the development of efficient, yet potentially very accurate, models to describe covalent and non-covalent (van der Waals) interactions in molecular systems. For chemical bonds, we use symmetrized force-based machine learning techniques that allow to achieve the "gold standard" quantum-chemical accuracy in the description of potential-energy surfaces of small and mid-sized molecules. For non-covalent interactions, we have developed coarse-grained quantum-mechanical models for interatomic potentials based on coupled harmonic oscillators. The accuracy, efficiency, and insight that can be obtained from both approaches will be demonstrated and future directions for integrating these models into next-generation quantum force fields for complex molecular systems will be discussed. All our developments are firmly motivated by challenging experimental observations, and we make connections to experiments throughout the talk.