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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 local chemical interactions, we have developed symmetrized force-based machine learning techniques that allow to achieve the "gold standard" quantum-chemical accuracy in the description of potential-energy surfaces of mid-sized molecules [1,2]. For non-covalent interactions, we have developed coarse-grained quantum-mechanical models for interatomic potentials based on coupled harmonic oscillators [3,4]. 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.

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[3] J. Hermann, R. A. DiStasio Jr., and A. Tkatchenko, Chem. Rev. 117, 4714 (2017).

[4] M. Stoehr, T. Van Voorhis, and A. Tkatchenko, Chem. Soc. Rev. 48, 4118 (2019).