Developing force-fields for complex materials: From novel catalytic materials to atmospheric processes to electrolytes for energy storage

TCI SEMINAR

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Recent advances in computational materials science have made ab initio/quantum simulations, at the density functional level, increasingly feasible from a computational standpoint. Unfortunately, the accessible length and time scales are still limited, of the order of a few nanometer in length and tens of picoseconds in time, necessitating the development of empirical models that can capture the structure and dynamics at significantly longer scales. The focus of my research is the development of these types of classical models or force-fields, from ab initio data, that are computationally efficient yet capture the essential physics of the problem. There are three main thrusts, namely, novel catalytic systems like metal organic frameworks, gas-liquid nucleation in the presence of acidic defects (relevant to atmospheric chemistry), and finally the study of novel electrolytes for next generation rechargeable battery technologies like sodium-air batteries. My talk will focus on the algorithm used to generate these force-fields and each of the three specific applications.

Theoretical Chemistry Institute Seminar Series