First-Principles Simulations of Electron Transport and Electrocatalysis of 2D Materials

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Computational methods based on quantum mechanics (first principles) are powerful tools to extract atomic-level understanding of materials and processes, which may be difficult to access experimentally. Here I will show two examples, where we develop and apply first-principles methods to understand (1) why 2D semiconductors generally have low electron mobility [1,2,3], and (2) the active site structure and kinetic mechanism of single metal atom embedded in graphene for electrochemical CO2 reduction and oxygen reduction [4,5].

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