



学术报告



Computational Materials Science and its Application in Structure Characterization of Hydrotalcite

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个人简历：

Hao Zhang is a professor at Alberta University. He received his bachelor's and master's degrees from Tsinghua University in 1996 and 1999 respectively., and then he received his Ph.D. in Mechanical and Aerospace Engineering from Princeton University in 2005. He was an assistant researcher at Princeton University from 2005-2007; an associate Professor at the University of Alberta from 2007-2017; and he has been a professor at the University of Alberta since 2017.



报告摘要：

In the first part of this talk, we will quickly review the major methodologies commonly employed in the computational materials science and briefly review a few research areas we have been working during the last ten years using molecular dynamics (MD) simulations. In the second part of this talk, we will be focusing on the application of MD simulations on the understanding of atomic structure of hydrotalcite. Hydrotalcite derived materials are considered to be promising candidates for solid sorbents for CO₂ capture at intermediate temperatures. Using MD simulation, we investigated the atomistic structures of monocarboxylic acid intercalated LDHs containing Mg and Al in the ratio of 3. The replacement of carbonate anions by stearate anions and the presence of water molecules could greatly increase the basal spacing. In addition, we investigated CO₂ adsorption behavior on amorphous layered double oxides (LDOs) derived from LDHs at elevated temperatures. The MD simulation of structure evolution upon heating agreed well with experimental results reported previously. The simulation results also showed that the CO₂ dynamic residence time on LDOs was sensitive to the Mg/Al molar ratio and the average amount of residence time of CO₂ on the surface of LDOs reached maximum when the Mg/Al molar ratio was equal to 3. Examination of the binding between CO₂ and mixed oxides revealed that both magnesium and oxygen in amorphous LDOs contributed to CO₂ adsorption.