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Ph.D. Student in Chemistry, admitted Summer 2018

Publications

PUBLICATIONS

• Characterizing and Contrasting Structural Proton Transport Mechanisms in Azole Hydrogen Bond Networks Using Ab Initio Molecular Dynamics. The journal of physical chemistry letters
  Atsango, A. O., Tuckerman, M. E., Markland, T. E.
  2021: 8749-8756

• Interfacial properties of pure and doped CdS/graphene composites: CdS (0001)/graphene and a CdS/graphene bilayer COMPUTATIONAL MATERIALS SCIENCE
  Bendavid, L., Atsango, A. O., Smith, R. W.
  2020; 177

• Elucidating the Proton Transport Pathways in Liquid Imidazole with First-Principles Molecular Dynamics. The journal of physical chemistry letters
  2020: 6156–63