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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