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Publications

PUBLICATIONS

• A two-directional vibrational probe reveals the distinct electric field orientation at the active site of liver alcohol dehydrogenase
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• Characterizing and Contrasting Structural Proton Transport Mechanisms in Azole Hydrogen Bond Networks Using Ab Initio Molecular Dynamics. The journal of physical chemistry letters
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• Interfacial properties of pure and doped CdS/graphene composites: CdS (0001)/graphene and a CdS/graphene bilayer
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• Elucidating the Proton Transport Pathways in Liquid Imidazole with First-Principles Molecular Dynamics. The journal of physical chemistry letters
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