



Summer Theory Workshop on Molecules and Materials: Design and Dynamics

Fri June 10, 2022, Smith Hall 206

10.00am: Steve Ndengué

ICTP-East African Institute for Fundamental Research, Kigali, Rwanda

Wavepacket studies of the water-dimer: New insights from 12D quantum dynamics

11.30am: Michele Pavanello

Electronic structure of molecular condensed phases from subsystem and orbital-free DFT approaches

2.00pm: Li Zhu

Metastable materials design through energy landscapes exploration

3.30pm: Neepa Maitra

Correlated dynamics of electrons, ions, and photons: TDDFT and the exact factorization approach

Sponsored in part by Department of Physics, Rutgers University Newark and the APS US-Africa Initiative