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Coupled Quantum Dynamics of Electrons and Protons: Multicomponent DFT extension of RT-TDDFT via nuclear-electronic orbital method

Wednesday, 13 January 2027 14:10 (0:30)

Content

Summary

Presenter(s) : YOSUKE KANAI (UNC Chapel Hill)

Session Classification : 2. Electrons and Phonons in the Time Domain: Excitations, Transport and Dynamics