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A molecular dynamics study of the relaxation of an excited benzene molecule chemisorbed to the surface of crystalline RDX ANDREY PEREVERZEV, THOMAS D. SEWELL, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211, ANDREI PIRYATINSKI, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87544 — Molecular dynamics simulations with a full-dimensional non-reactive potential-energy surface were used to study energy transfer from an excited benzene molecule covalently bonded to the surface of RDX crystal at 298 K and atmospheric pressure. The crystal is treated as a periodic, freestanding thin film approximately 5 nm thick. Initial conditions for the excited molecule were obtained from quantum mechanical calculations. Dominant energy redistribution pathways both in the space of atomic coordinates and in the space of crystal normal modes will be reported. Theoretical models of energy relaxation processes in this and similar systems will be discussed.

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