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Importance of Electronic Relaxation for Inter-Coulombic Decay in Aqueous Systems[1] DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory (LBNL), CRAIG P. SCHWARTZ, RICHARD J. SAYKALLY, Chemistry Dept., University of California, Berkeley and Chemical Sciences, LBNL, SHERVIN FATEHI, Kenneth S. Pitzer Center for Theoretical Chemistry, University of California, KEITH V. LAWLER, Chemical Sciences, LBNL, C. WILLIAM MCCURDY, Chemical Sciences, LBNL and Departments of Applied Science and Chemistry, University of California, Davis — Inspired by recent photoelectron spectroscopy experiments on hydroxide solutions, we have examined the conditions necessary for enhanced (and, in the case of solutions, detectable) intermolecular Coulombic decay (ICD) – Auger emission from an atomic site other than that originally excited. We present general guidelines, based on energetic and spatial overlap of molecular orbitals, for this enhancement of ICD-based energy transfer in solutions. These guidelines indicate that this decay process should be exhibited by broad classes of biomolecules and suggest a design criterion for targeted radiooncology protocols. Our findings indicate that ICD processes in hydroxide solutions are not dependent on hydroxide hydrogen bond donation.

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