Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

Real-Time Tracking of Interfacial Charge Dynamics in a Metal–Dielectric Janus Nanocluster

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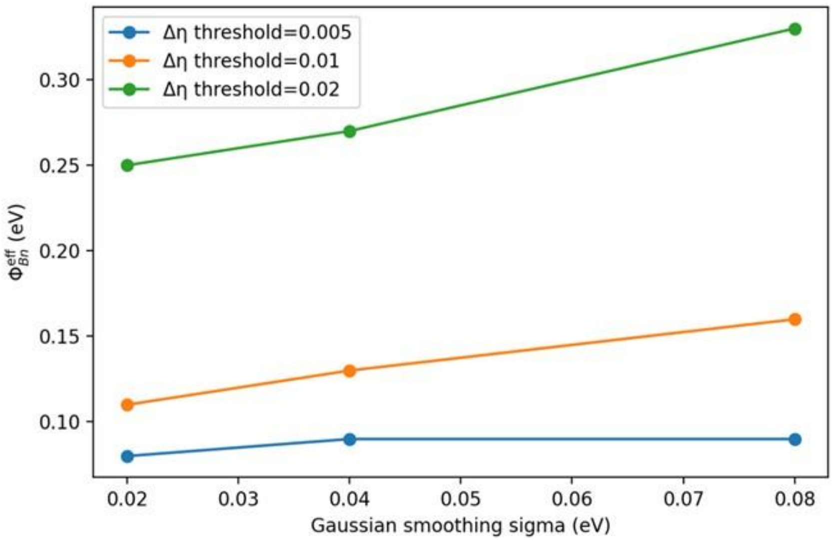

Figure S1. Dependence of the effective electron injection barrier, $\Phi_B{}^{\mathrm{eff}}{}_{n'}$ on the excess injection threshold $\Delta\eta$ and Gaussian spectral broadening σ. The extracted barrier shows weak sensitivity to σ over the range $0.02 - 0.08$eV.

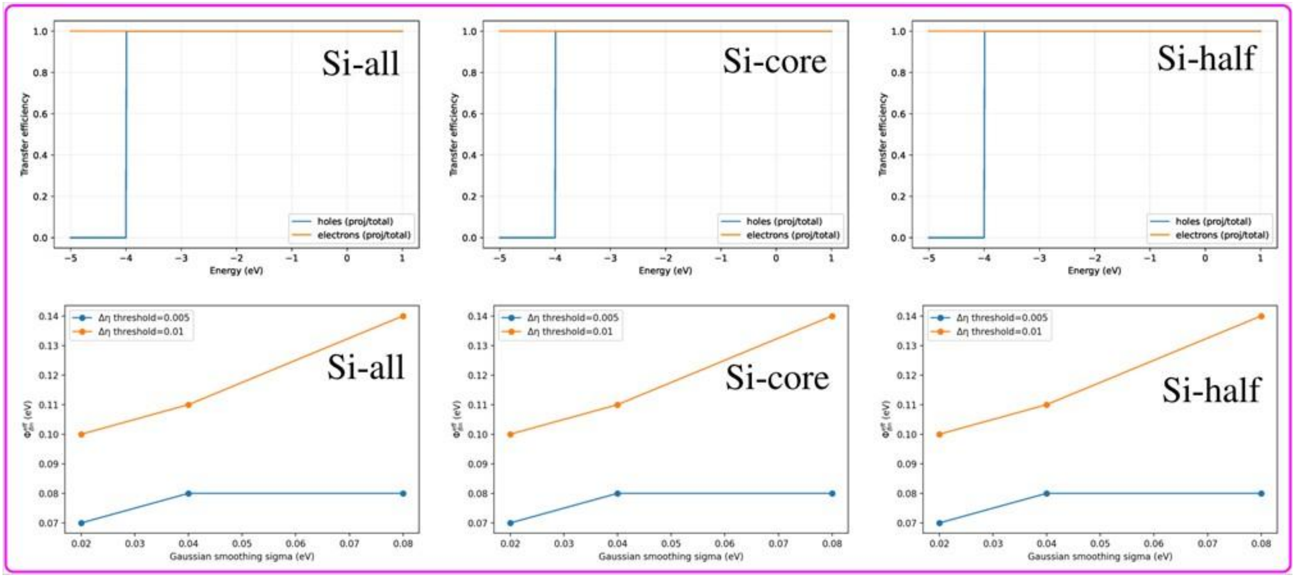

Figure S2. Transfer efficiency and effective injection barrier $\Phi_{Bn}{}^{\mathrm{eff}}$ evaluated for different Si partitioning schemes (Si-all, Si -core, and Si -half), showing consistent near-Fermi injection behavior across partition choices.

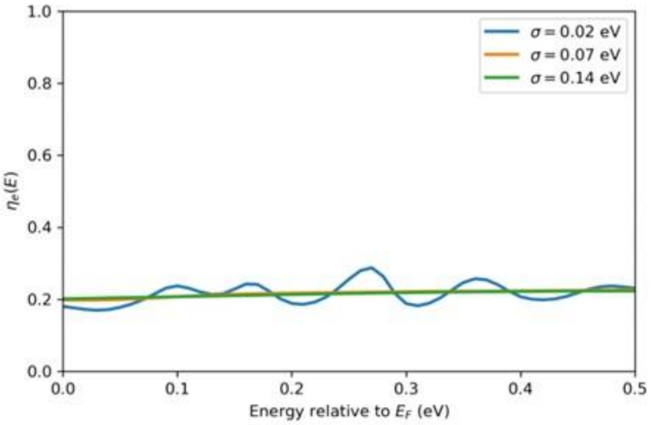

Figure S3. Si-resolved electron population $n_e(E)$ above E_F for different Gaussian broadenings ($\sigma = 0.02 - 0.14\text{eV}$), showing robust near-Fermi injection.

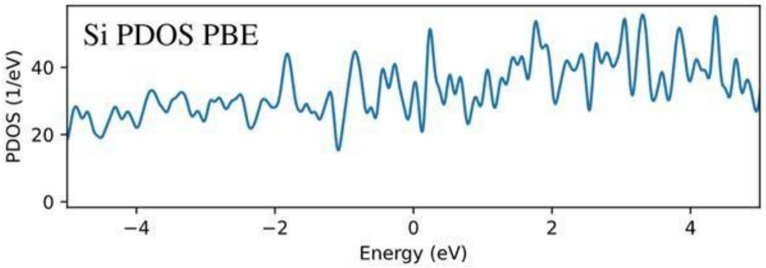

Figure S4. Si-projected density of states computed using the PBE functional.

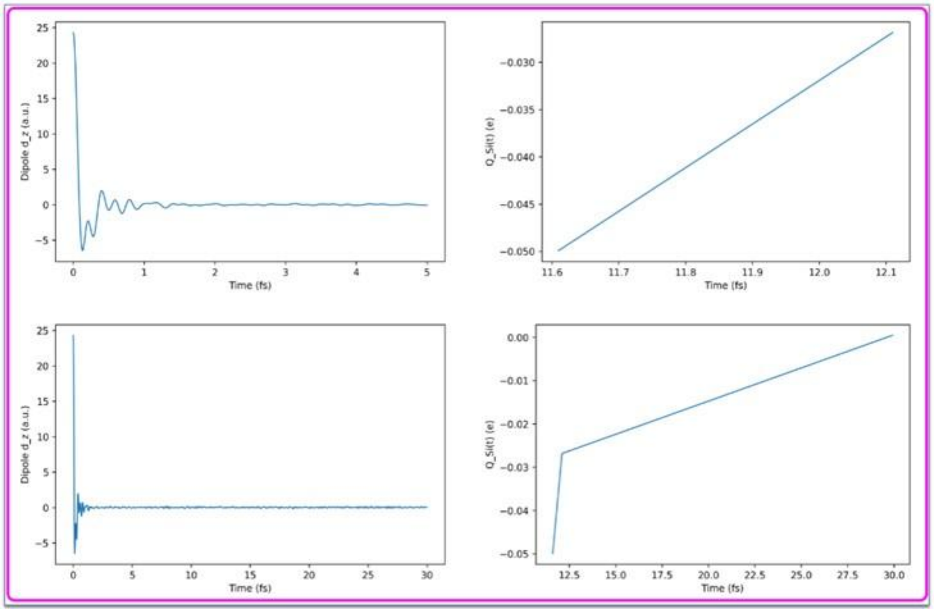

Figure S5. Time-resolved dipole moment and Si charge dynamics showing early-time coherent oscillations and subsequent electronic dephasing.

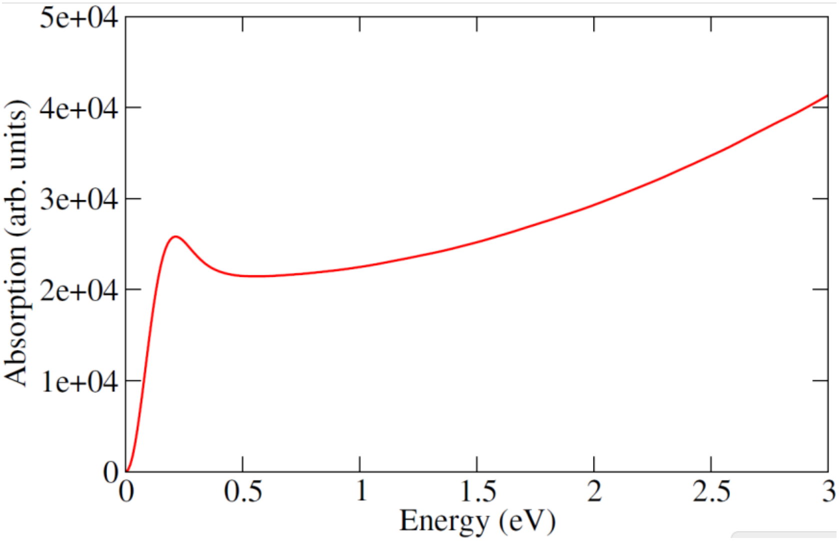

Figure S6. Absorption spectrum.