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Probing the Surface-to-Bulk Transition: A Closed-Form, Constant-Scaling Algorithm for Computing Subsurface Green Functions MATTHEW REUTER, Department of Chemistry, Northwestern University, TAMAR SEIDEMAN, MARK RATNER — A closed-form algorithm for computing subsurface Green functions—the blocks of a material's Green function between the surface and the bulk—is presented, where we assume the system satisfies a common principal layer approximation. By exploiting the block tridiagonal and nearly block Toeplitz structure of the Hamiltonian and overlap matrices, this method scales independently of the system size (constant scaling), allowing studies of large systems. As a proof-of-concept example, we investigate the decay of surface effects in an armchair graphene nanoribbon, demonstrating the persistence of surface effects hundreds of atomic layers ($\sim$0.5 μm) away from a surface. We finally compare the surface-to-bulk transitions of finite and semi-infinite systems, finding that finite systems exhibit amplified surface effects.

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