First-principles study of the excited-state properties of Tryptophan in water

JE-LUEN LI, Princeton University, J.B. NEATON, PAUL TANGNEY, The Molecular Foundry, LBNL and Department of Physics, UC Berkeley, NED S. WINGREEN, Department of Molecular Biology, Princeton University, ROBERTO CAR, Department of Chemistry, Princeton University, STEVEN G. LOUIE, The Molecular Foundry, LBNL and Department of Physics, UC Berkeley

— Tryptophan (Trp) is an optically-active amino acid that is highly sensitive to its local environment and responsible for much of the UV fluorescence in proteins. The spectral properties of Trp are primarily associated with the two low-lying excited states, $^1L_a$ and $^1L_b$, of its indole side chain. These states possess strong dipole moments and give rise to a complex excited-state relaxation dynamics in polar solvents like water. Here we apply first-principles calculations to examine the impact of the surrounding solution on the indole excited states responsible for UV fluorescence. Results of excited-state calculations of molecular indole using the GW-Bethe Salpeter equation (GW-BSE) formalism will be presented and compared with existing quantum-chemical calculations. Results of ground- and excited-state molecular dynamics simulations will also be presented.

Je-Luen Li
Princeton University