Abstract Submitted
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First principles theory for surface plasmon generation and decay to hot carriers[1] RAVISHANKAR SUNDARARAMAN, PRINEHA NARANG, ADAM JERMYN, HARRY A. ATWATER, WILLIAM A. GODDARD III, Joint Center for Artificial Photosynthesis — Plasmonic resonances provide a promising pathway for efficiently capturing infrared photons from solar radiation and boosting photo-catalytic activity via local temperature enhancements and hot carrier generation. Previous calculations of plasmon decay to excited carriers employing a fully quantized model Hamiltonian [2] indicate strong plasmon polarization dependence and momentum anisotropy of the generated carriers, in contrast with classical theories. An accurate first principles calculation for this process must account for microscopic details at the atomic scale for the electronic states as well as the effect of the 10-100 nm length scale particle and antennae geometries on the plasmon resonances. Here, we present a first-principles multi-scale model of plasmonics combining electronic density-functional theory with electromagnetic models on longer length-scales, and investigate the role of electronic structure and geometry on plasmonic light absorption, decay and hot carrier generation.

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[2]A. Jermyn, P. Narang and H. A. Atwater, *(under preparation)*

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