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Excited carrier dynamics and transport in plasmonic nanostructures[1] RAVISHANKAR SUNDARARAMAN, PRINEHA NARANG, ADAM JERMYN, HARRY ATWATER, WILLIAM GODDARD III, Joint Center for Artificial Photosynthesis, California Institute of Technology — Surface plasmon resonances provide a pathway to efficiently capture electromagnetic radiation in sub-wavelength structures for energy conversion and photodetection at the nano scale. The complete mechanism involves several microscopic steps spanning length scales from atomic dimensions to tens or hundreds of nanometers, posing challenges for experimental characterization and for first-principles predictions. To provide the basis for predicting and optimizing the complex interplay of materials and geometric effects in plasmon decay-induced excited carrier phenomena, we combined *ab initio* electronic structure calculations, electromagnetic simulations and Boltzmann transport models. In Au, Ag, Cu and Al nanostructures, we find that initial carrier distributions as well as their subsequent transport, relaxation and thermalization are sensitive to electronic structure, exhibiting strong asymmetries between electrons and holes. We predict energy-dependent spatially-resolved carrier distributions collected in plasmonic nanostructures with strong field inhomogeneities, and explore the possibility of tailoring materials and geometry to collect the carrier distributions needed for such applications as photochemically driven CO_2 reduction and water splitting.

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