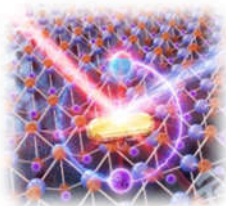


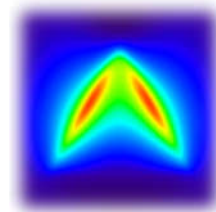
## Building and testing semiclassical models for molecular plasmonics



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Molecular plasmonics has been a hot topic for the past several years. At the heart of the primary interest in plasmonics is the strong electromagnetic field localization at resonant frequencies corresponding to surface plasmon-polariton modes. Thanks to riveting advancements in nanofabrication technologies, we have achieved nearly 1 nm spatial resolution (and in some cases even below that!) and are able to fabricate a wide variety of nanosystems ranging from nanoparticles of various shapes to metasurfaces comprised of periodic arrays of nanoparticles and/or nanoholes of any imaginable geometry. Such systems have recently emerged as new platforms for strong light-matter interactions. Combined with molecular ensembles, these constructs exhibit a remarkable set of optical phenomena ranging from the exciton-plasmon strong coupling to the second harmonic generation altered by molecular resonances. In this talk I will discuss both linear and nonlinear optical properties of plasmonic materials coupled to quantum emitters of various complexity. I will also introduce a newly developed computational approach that can be used to efficiently simulate a large number of complex molecules driven by electromagnetic radiation crafted at plasmonic interfaces.

### Representative publications:

1. “Efficient parallel strategy for molecular plasmonics – a new numerical tool for Maxwell-Schrödinger equations in three dimensions”, M. Sukharev, *Journal of Computational Physics* **477**, 111920 (2023).
2. “Dissociation slowdown by collective optical response under strong coupling conditions”, M. Sukharev, J. Subotnik, A. Nitzan, (Editor’s Choice) *Journal of Chemical Physics* **158**, 084104 (2023).
3. “Fano plasmonics goes nonlinear”, M. Sukharev, E. Drobnih, R. Pachter, *Journal of Chemical Physics* **157**, 134105 (2022).
4. “Second harmonic generation by strongly coupled exciton-plasmons: the role of polaritonic states in nonlinear dynamics”, M. Sukharev, A. Salomon, J. Zyss, *Journal of Chemical Physics* **154**, 244701 (2021).
5. “Second harmonic generation from a single plasmonic nanorod strongly coupled to a WSe<sub>2</sub> monolayer”, C. Li, X. Lu, A. Srivastava, S. D. Storm, R. Gelfand, M. Pelton, M. Sukharev, H. Harutyunyan, *Nano Letters* **21**, 1599 (2020).
6. “Plasmon enhanced second harmonic generation by periodic arrays of triangular nanoholes coupled to molecular emitters”, E. Drobnih and M. Sukharev, *Journal of Chemical Physics* **152**, 094706 (2020).
7. “Energy transfer and interference by collective electromagnetic coupling”, M. Gómez-Castaño, A. R. Cubero, L. Buisson, J. L. Pau, A. Mihi, S. Ravaine, R. A. L. Vallée, A. Nitzan, M. Sukharev, *Nano Letters* **19**, 5790 (2019).