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Title: Voltage-Driven Long Exciton Lifetimes and Strong Light–Matter Coupling in STM Break Junctions

Abstract: Scanning tunneling microscope break junction (STM-BJ) systems have recently demonstrated strong light–matter coupling at the single-molecule level, reaching values up to 300 meV, despite their typically lossy nanocavities. Unlike laser-driven platforms, STM-BJ systems excite molecules through an applied voltage, with specific voltages significantly enhancing electroluminescence efficiency. To understand the mechanisms behind this behavior, we employ ab initio methods, including both real-time and linear response time-dependent density functional theory (TDDFT), Maxwell simulations and model analyses based on the Newns–Anderson framework. Our study examines exciton lifetimes, electromagnetic mode structures, and mode volumes under voltage- versus laser-driven excitation. We identify optimal field conditions that simultaneously improve exciton lifetimes and enhance mode confinement. These insights suggest new design principles for achieving and controlling strong coupling in plasmonic nanocavities.