Plasmons in quasi-two-dimensional metals

12.1.6: Van der Waals bonding in advanced materials (DMP)

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We employ ab initio density-functional theory (DFT) and GW calculations to understand and predict the plasmon dispersion in quasi-two-dimensional (quasi-2D) metals. We show that, unlike what is found in idealized 2D electron gases, plasmons are virtually dispersionless in real quasi-2D metals for a wide range of excitation wave vectors that are experimentally accessible. We further develop a simpler model that captures this plasmon dispersion in quasi-2D metals and which depends on a single parameter: the characteristic screening length due to interband transitions. Our ab initio calculations further predict that monolayer metallic transition metal dichalcogenides are excellent candidates to explore these dispersionless (flat) plasmons: having large excitation energy that is away from the Landau damping regions makes them ideal systems to support long-lived, spatially-localized 2D plasmons which are highly tunable with substrate. This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, and by the National Science Foundation.