Localized surface plasmon resonances and electric field confinement in titanium carbide (Ti_3C_2) MXene nanoclusters

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Abstract: Two-dimensional metal carbides and nitrides, known as MXenes, are an emerging class of materials that are promising for a variety of applications. In this work, using time-dependent density functional theory calculations, we investigate the localized surface plasmon resonances and electric field confinement of pristine and surface-terminated [fluorinated (F) and/or oxidized (O)] mono-layered titanium carbide (Ti_3C_2) MXene nanoclusters. We found that the nanoclusters ($Ti_{48}C_{32}$, $Ti_{48}C_{32}F_{32}$, and $Ti_{48}C_{32}O_{32}$) exhibit broadband photoabsorption spectra and localized surface plasmon resonances even at low energy in the infrared region (a spectral range of interest for molecular sensing). In addition, the nanoclusters produce a sizable electric field confinement on the surface with a strength that varies with the F/O surface termination. Our findings provide significant theoretical insight into the optical and plasmonic properties of MXene nanoclusters.