Molecule-Induced Conformational Change in Two-Dimensional Nanomaterials with Enhanced Surface Adsorption

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Abstract Boron nitride (BN) nanosheets have been proven to be excellent adsorbent of aromatic molecules via π - π interaction. Our density functional theory (DFT) calculations and experimental measurements using Raman spectroscopy reveal that BN nanosheets, as well as other two-dimensional nanomaterials, could adjust their morphology to accommodate physisorbed molecules, resulting in larger interaction energies and higher adsorption capability than bulk crystal BN. This unique property leads to many new applications. For example, BN nanosheets can enable highly sensitive, stable, reproducible, and reusable surface enhanced Raman spectroscopy (SERS) substrates. BN nanosheet can increase the sensitivity of plasmonic metal particles by 2 orders. Due to excellent thermal stability, flexibility and impermeability of BN nanosheets, the substrate could be reused without essential loss of plasmon enhancement.

Figure



Figure 1. Intensity changes of rhodamine 6G Raman signal at 610 cm⁻¹ from three different substrates under reusability test.