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A novel sensitive and stable surface enhanced Raman scattering substrate based on MoS_2 quantum dots/reduced graphene oxide hybrid system

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The calculation of the EF values :

The peak at 614 cm^{-1} of the inplane vibration of the ring was chosen for calculation of the enhancement factor because it is isolated from interference with nearby lines. The substrate enhancement factor is given by equation (1):

$$EF = \frac{I_{SERS} \times N_{Raman}}{I_{Raman} \times N_{SERS}} \qquad (1)$$

I is the corresponding intensity of the line selected. N is the number of molecules sampled by the laser spot. Using the probe spot size of the laser which is 10 μm in diameter (5 μm radius), the path length in the liquid of about 1 cm, and the number of

molecules (N_{Raman}) in the bulk R6G with the concentration of 0.0001 M can be obtain. According to the surface coverage of molecules and the laser spot size, the N_{SERS} can be gained by calculation. The intensity ratio of I_{SERS}/I_{Raman} can be calculated from the observed spectra. Factor calculated for other line is similar.

Theoretical Modeling and Calculations :

All the calculations performed in this work are carried out by using the VASP code,[1,2] where the rojector augmented wave (PAW) pseudopotentials and the Perdew-Burke-Ernzerh of (PBE)[3] exchange-correlation functional within the generalized gradient approximation (GGA) are adopted. The electronic wave functions are described by a set of plane wave functions with an energy cutoff of 400 eV. The convergence criterions for energy and force on each atom are 1.0×10^{-5} eV and 0.02 eV/Å, respectively. The T-MoS_2 quantum dot is constructed as shown in Fig.S1 with the stoichiometry of $Mo_{13}S_{26}$. After fully relaxed, this quantum dot is almost circular. Then, this quantum dot is placed on the center of the graphite supercell, which contains 8×8×1 unit cells of graphite. The Brillouin zones are sampled by a 4×4×1 Γ-centered k-point mesh within the Monkhorst-Pack cheme.

1. G. Kresse and J. Hafner, Phys. Rev. B, 1993, 47, 558.

2. G. Kresse and J. Furthmuller, Phys. Rev. B 1996, 54, 11169.

3. J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 1996, 77, 3865.

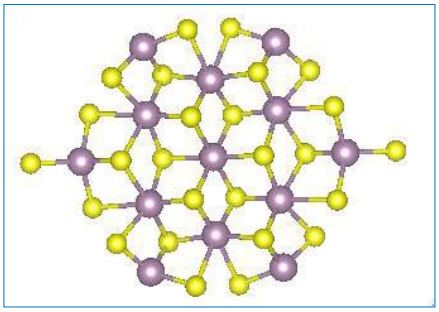

Fig.S1 the optimized structure of MoS_2 QDs.

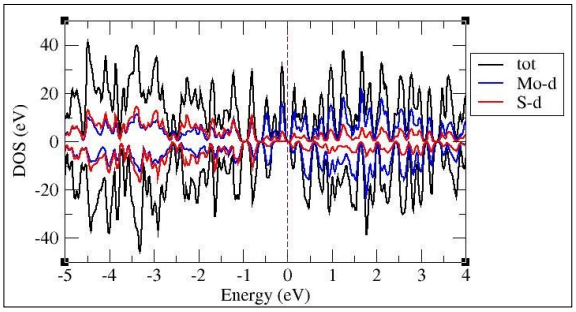

Fig.S2 the density of states of MoS_2 QDs.