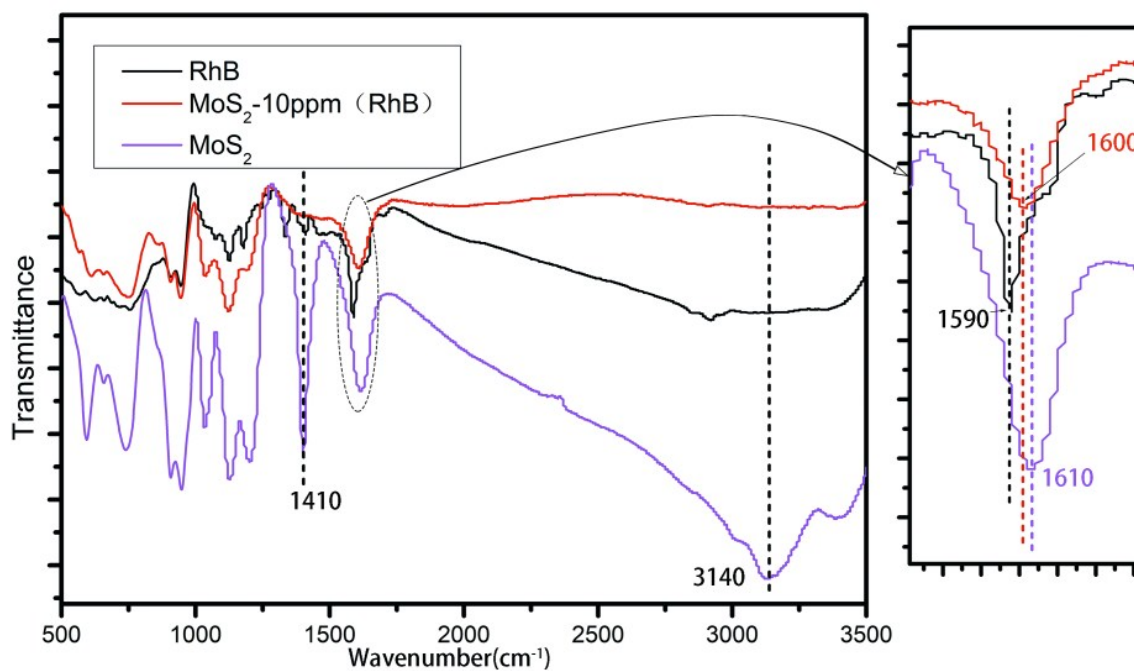


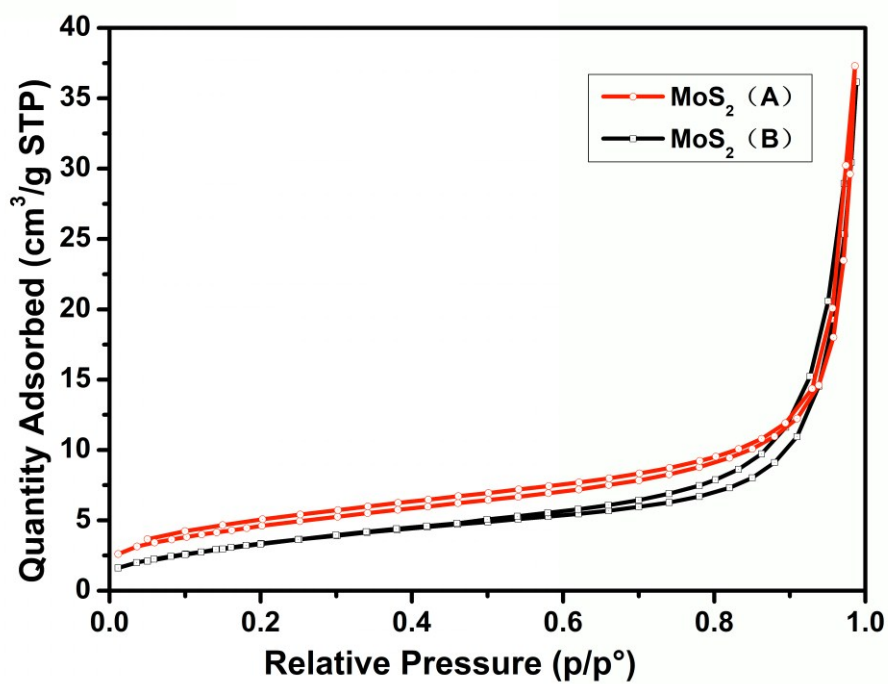
**Table S1** MoS<sub>2</sub> samples and SERS effect

| RhB                  | Van der Waals interaction |            |            | C=C and C=O bonds coordination |            |            | -NH <sub>2</sub> coordination |            |            |
|----------------------|---------------------------|------------|------------|--------------------------------|------------|------------|-------------------------------|------------|------------|
|                      | 10ppm                     | 1ppm       | 0.1ppm     | 10ppm                          | 1ppm       | 0.1ppm     | 10ppm                         | 1ppm       | 0.1ppm     |
| MoS <sub>2</sub> (A) | Yes<br>(✓)                | Yes<br>(×) | Yes<br>(×) | Yes<br>(✓)                     | Yes<br>(✓) | Yes<br>(×) | Yes<br>(✓)                    | Yes<br>(✓) | Yes<br>(✓) |
| MoS <sub>2</sub> (B) | Yes<br>(✓)                | Yes<br>(×) | Yes<br>(×) | Yes<br>(✓)                     | Yes<br>(✓) | Yes<br>(×) | No<br>(×)                     | No<br>(×)  | No<br>(×)  |
| MoS <sub>2</sub> (C) | Yes<br>(✓)                | Yes<br>(×) | Yes<br>(×) | No<br>(×)                      | No<br>(×)  | No<br>(×)  | No<br>(×)                     | No<br>(×)  | No<br>(×)  |

Illustration: 1) Yes or No suggests there exist this kind of interaction or not  
 2) (✓) or (×) means this interaction is contributes to the SERS effect or not



**Figure S1** FT-IR spectra of MoS<sub>2</sub>, MoS<sub>2</sub>-10ppm RhB and RhB



**Figure S2** N<sub>2</sub> adsorption-desorption isotherms of MoS<sub>2</sub>(A) and MoS<sub>2</sub>(B)

The BET surface area of MoS<sub>2</sub>(A) is 16.7632±0.0730 m<sup>2</sup> /g, and after annealing: 12.9093±0.1372 m<sup>2</sup> /g. That is, the annealing process reduced the specific surface area of MoS<sub>2</sub> by about 25%, and the reduction was not enough to cause a huge change of SERS effect.