

Comparative study of CO adsorption on Au, Cu, MoO₂ and MoS₂ 2D Nanoparticles

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Table I: Interatomic distances of Au, Cu, MoO₂ and MoS₂,
Quantum Espresso(QE), Gaussian

| Construction | Topology | distance(QE) | distance(Gaussian) |
|------------------|----------|---------------------------------------|---------------------------------------|
| Au | 10 | 2.72, 2.63 | 2.76, 2.71 |
| | 12 | 2.69, 2.71 | 2.73, 2.75 |
| | 14 | 2.60, 2.69 | 2.65, 2.63 |
| Cu | 10 | 2.38, 2.39 | 2.39, 2.58 |
| | 12 | 2.37, 2.38 | 2.44, 2.47 |
| | 14 | 2.38, 2.30 | 2.41, 2.46 |
| MoO ₂ | 10 | Mo-Mo: 2.58, 2.76 Mo-O: 2.55, 2.79 | Mo-Mo: 2.51, 2.79 Mo-O: 2.44, 2.83 |
| | 12 | Mo-Mo: 2.90, 2.79 Mo-O: 1.88, 2.05 | Mo-Mo: 2.90, 2.73 Mo-O: 1.90, 2.02 |
| | 14 | Mo-Mo: 2.67, 2.60 Mo-O: 1.88, 2.03 | Mo-Mo: 2.68, 2.84 Mo-O: 1.99, 2.03 |
| | 10 | Mo-Mo: 2.29, 3.04 Mo-S: 2.23, 2.53 | Mo-Mo: 2.90, 2.91 Mo-S: 2.45, 2.38 |
| MoS ₂ | 12 | Mo-Mo: 3.02, 2.97 Mo-S: 2.36, 2.39 | Mo-Mo: 3.11, 2.97 Mo-S: 2.32, 2.42 |
| | 14 | Mo-Mo: 2.94, 2.87 Mo-S: 2.33, 2.44 | Mo-Mo: 3.09, 2.82 Mo-S: 2.26, 2.39 |

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