

Electronic Supplementary Information:

Simultaneous adsorption of SO₂ and CO₂ in metal-organic framework Ni(bdc)(ted)_{0.5}

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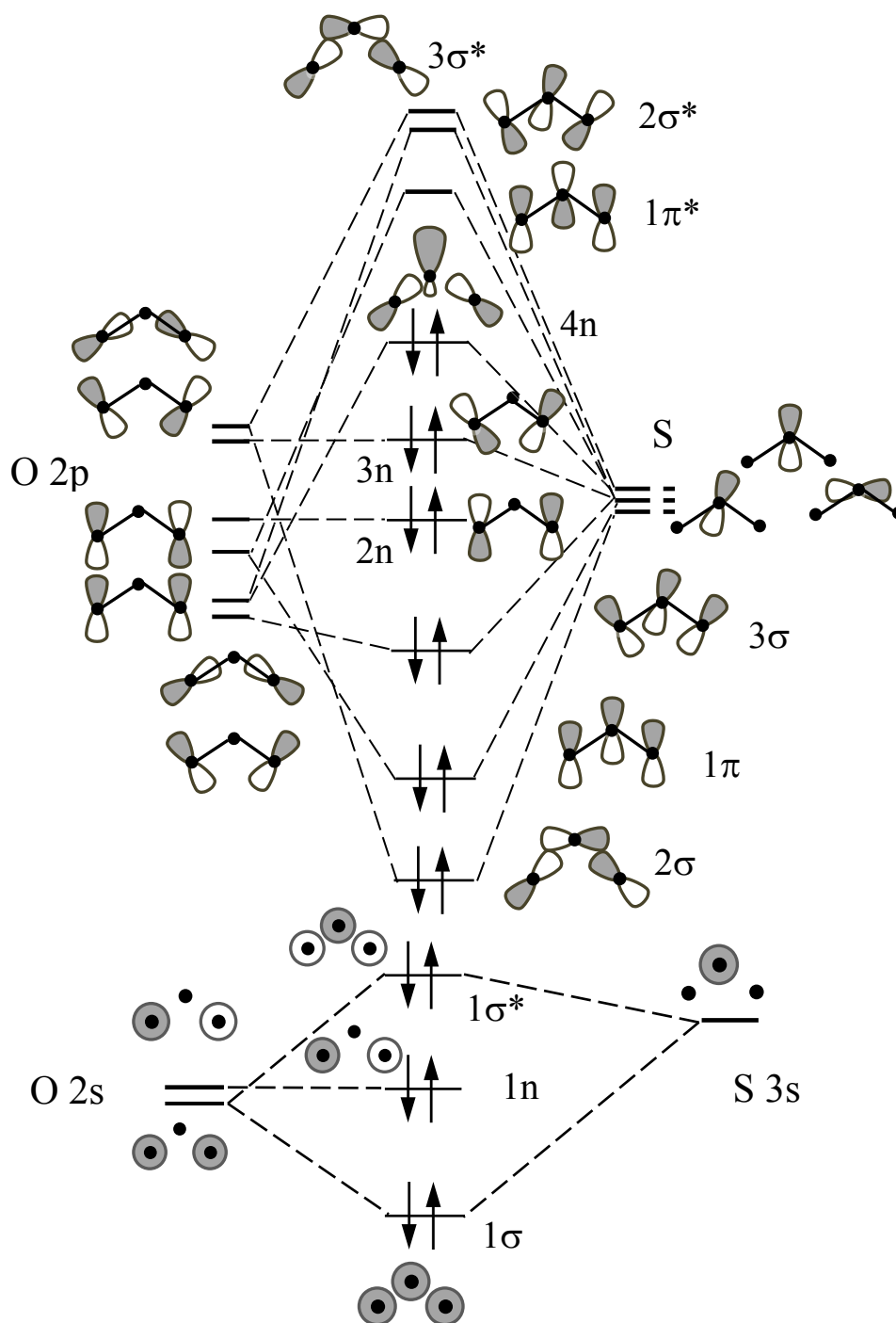
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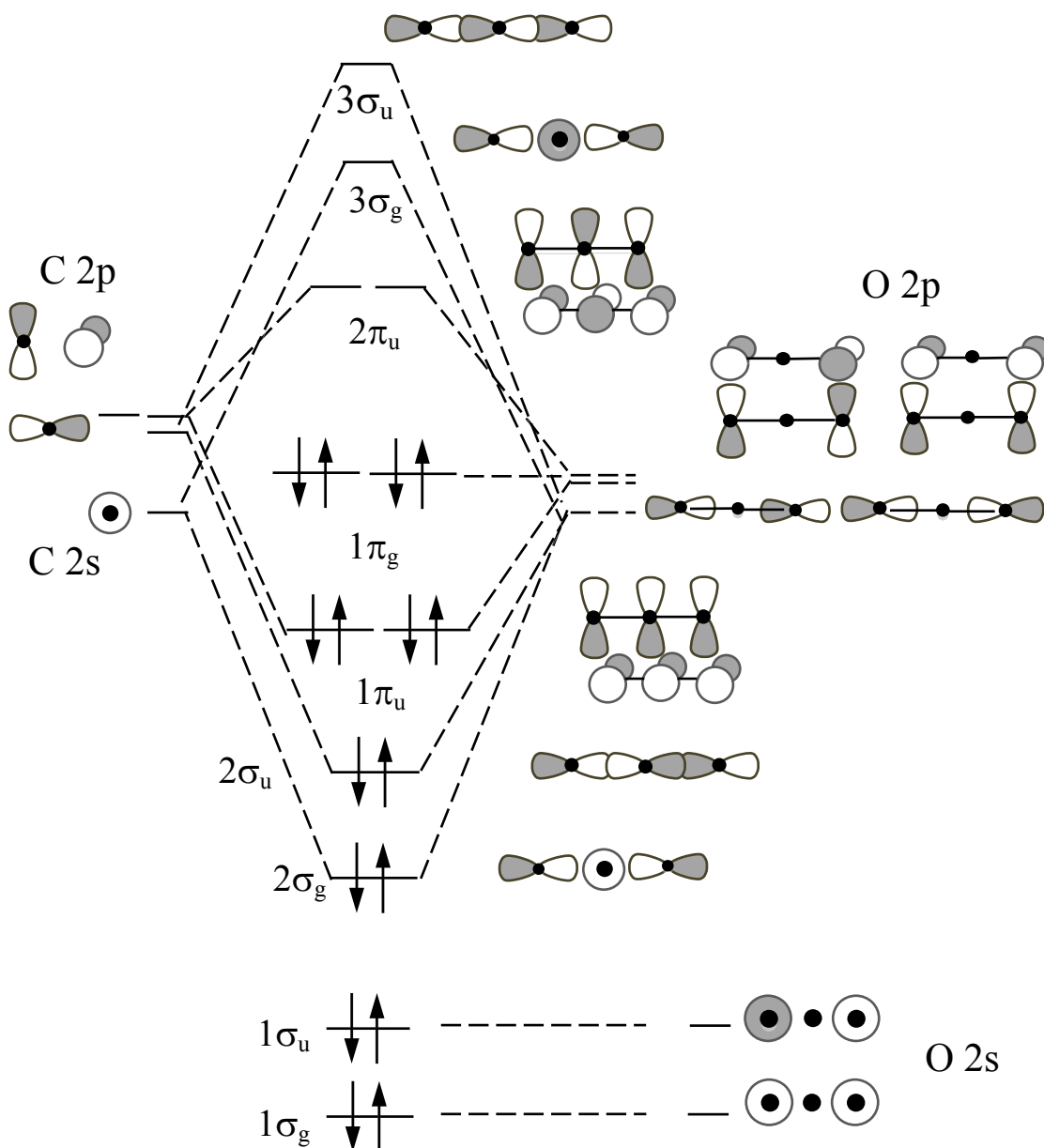
1. Molecular orbital diagram for SO₂.
2. Molecular orbital diagram for CO₂.

1. Molecular orbital diagram for SO₂



Scheme S1. Molecular orbital diagram for SO₂. The $4n$ state is the combination of the sp^2 hybridization of the sulfur and the p orbitals of the oxygen atoms. This state corresponds to the highest occupied molecular orbital (HOMO) in the DOS of SO₂. The $3n$ and $2n$ states are the non-bonding states of the oxygen atoms, and the $1\pi^*$ state is the anti-bonding state which corresponds to the lowest unoccupied molecular orbital (LUMO) in the DOS of SO₂.

2. Molecular orbital diagram for CO₂



Scheme S2. Molecular orbital diagram for CO₂. The 1π_g states is the non-bonding states of CO₂ which correspond to the lone pairs of the oxygen atoms. The non-bonding states correspond to the HOMO in the DOS of CO₂. The 1π_u states are the anti-bonding states which correspond to the LUMO of CO₂.