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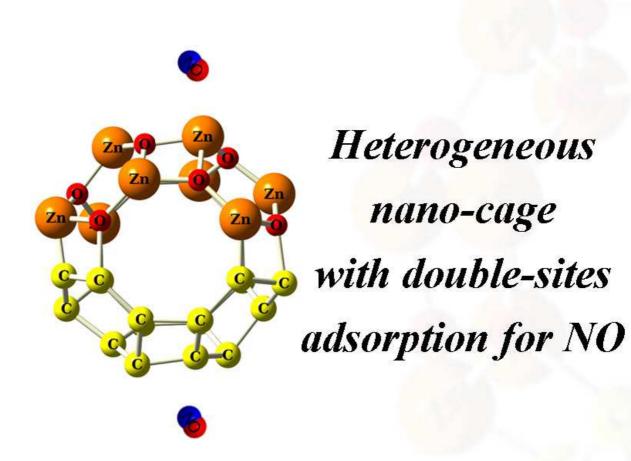
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- Adsorption of NO molecule was investigated on the surface of a novel heterogeneous C₁₆Zn₈O₈ nano-cluster.
- Full optimization for all configurations revealed that the NO molecule was adsorbed on the both ZnO and C surface of nano-cluster.

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