

Computational modeling of a prototypical photocatalyst: a zeolite encapsulated TiO_2 -supported Cu_5 cluster

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Sabelo A. Cele

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Inspireer uitnemendheid. Verander lewens*

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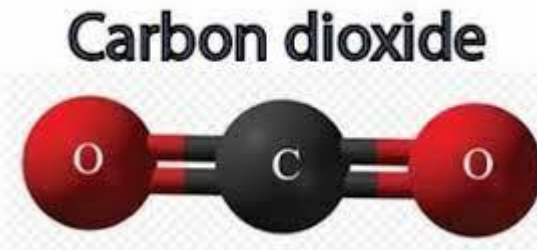
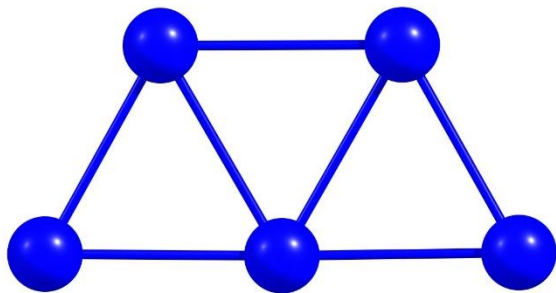
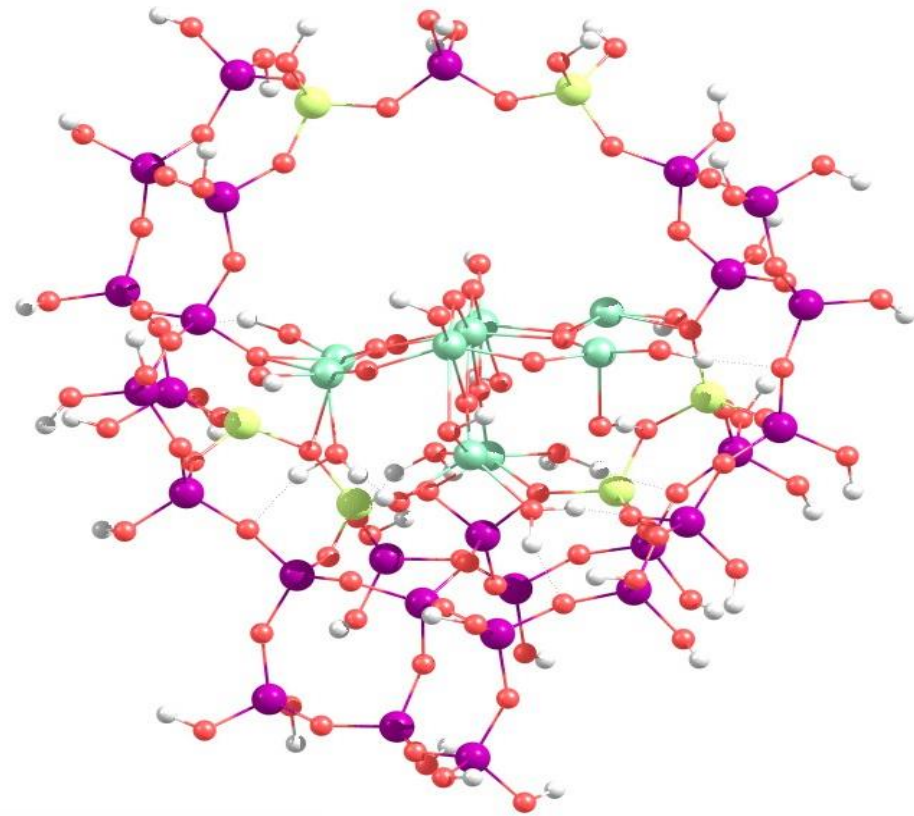
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Background

- This is a theoretical study.
- This photocatalyst consists of the following:
 - ❖ Zeolite Y
 - ❖ Rutile TiO_2 (110)
 - ❖ Cu_5 cluster
 - ❖ CO_2
- The motive of the project is to study the reduction of CO_2 to CO and O



Methodology

DFT Calculations

- Orca software
- Geometry Optimisation
- Single Point Calculation

Basis Set

- SVP (normal/double)
- SVP/TZVPP (dual)

D3BJ (dispersion correction)

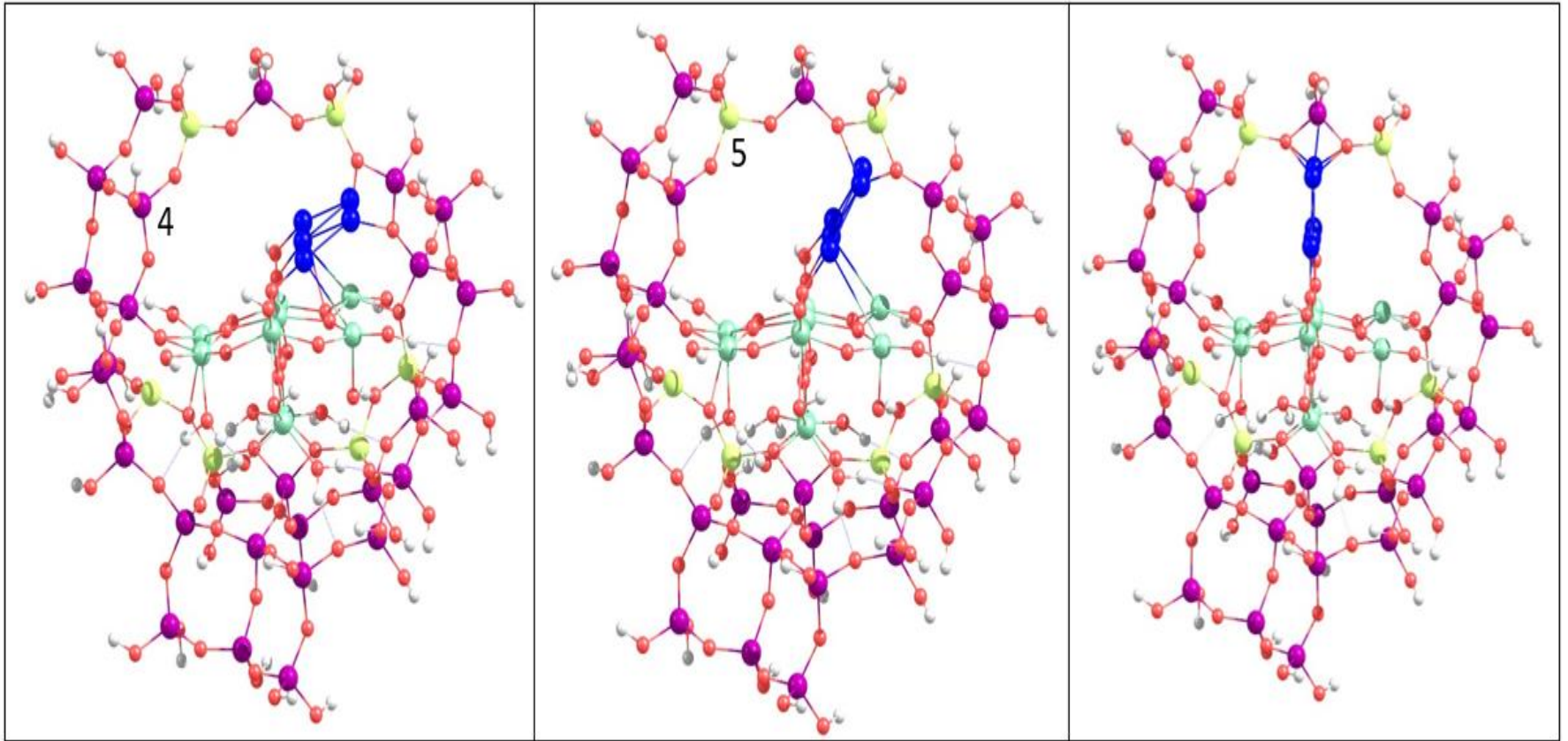
Constraints

- Zeolite (TiO_2 & Cu_5 opt)
- Zeolite & TiO_2 (Cu_5 opt)

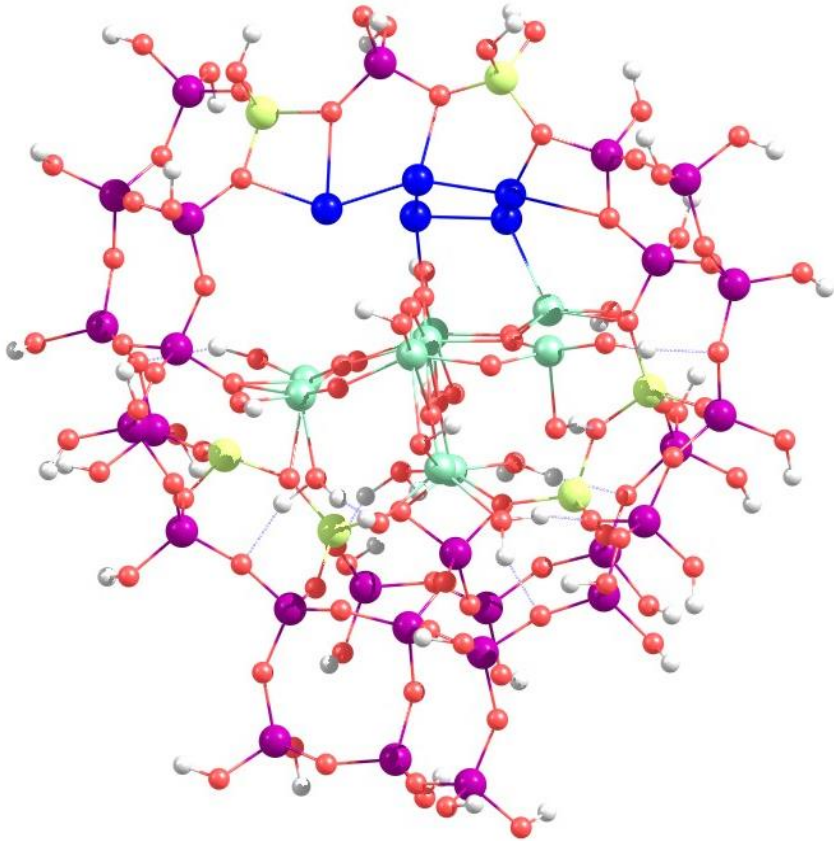
PBE function

Charge is 0

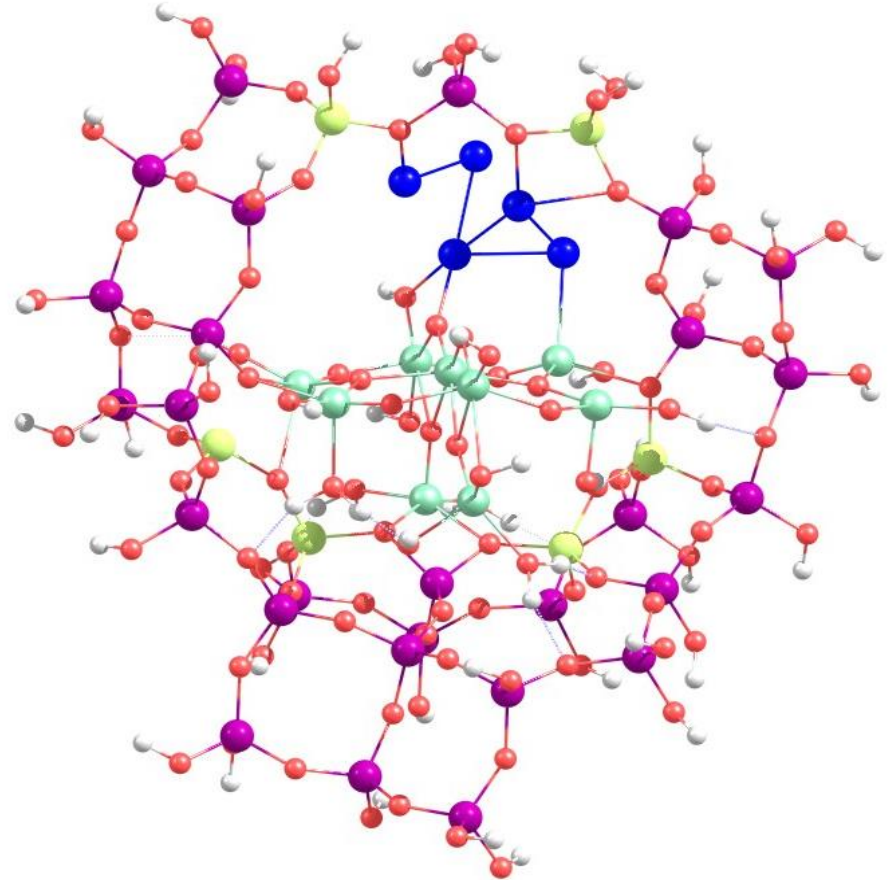
Spin multiplicity is 2



Results



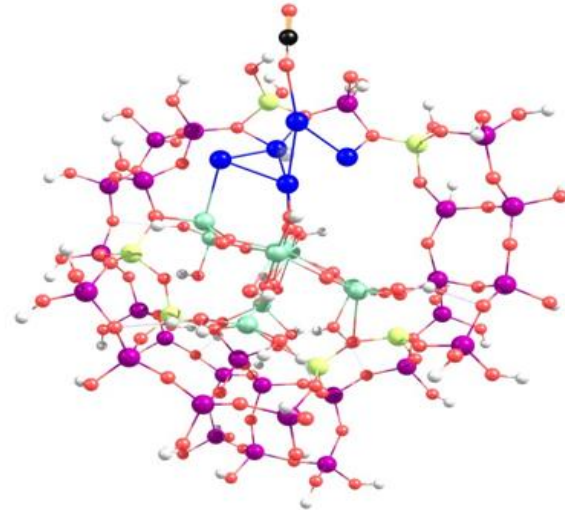
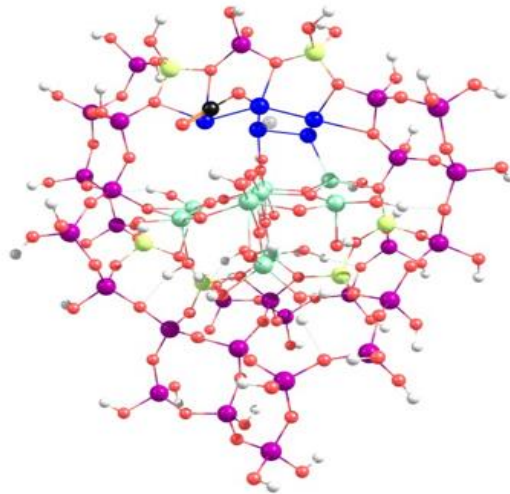
1



2

Results

CO₂



CO-O

