

## Supplementary Information

### CO<sub>2</sub> adsorption on gas-phase Cu<sub>4-x</sub>Pt<sub>x</sub> (x = 0 - 4) clusters: a DFT study

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**Figure SI1 (a).** Transition state energy barrier calculated using the linear synchronous transit (LST) method between the planar rhombus Cu<sub>4</sub> cluster and the planar y-shaped Cu<sub>4</sub> cluster.

**Figure SI1 (b).** Transition state energy barrier calculated using the linear synchronous transit (LST) method between the 3D pyramidal Cu<sub>1</sub>Pt<sub>3</sub> cluster and the planar rhombus Cu<sub>1</sub>Pt<sub>3</sub> cluster.

**Figure SI1 (c).** Transition state energy barrier calculated using the linear synchronous transit (LST) method between the 3D pyramidal Cu<sub>2</sub>Pt<sub>2</sub> cluster and the planar rhombus Cu<sub>2</sub>Pt<sub>2</sub> cluster.





