Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Exploring Si-Centered Phthalocyanine as a single atom catalyst for N_2O reduction: a DFT study

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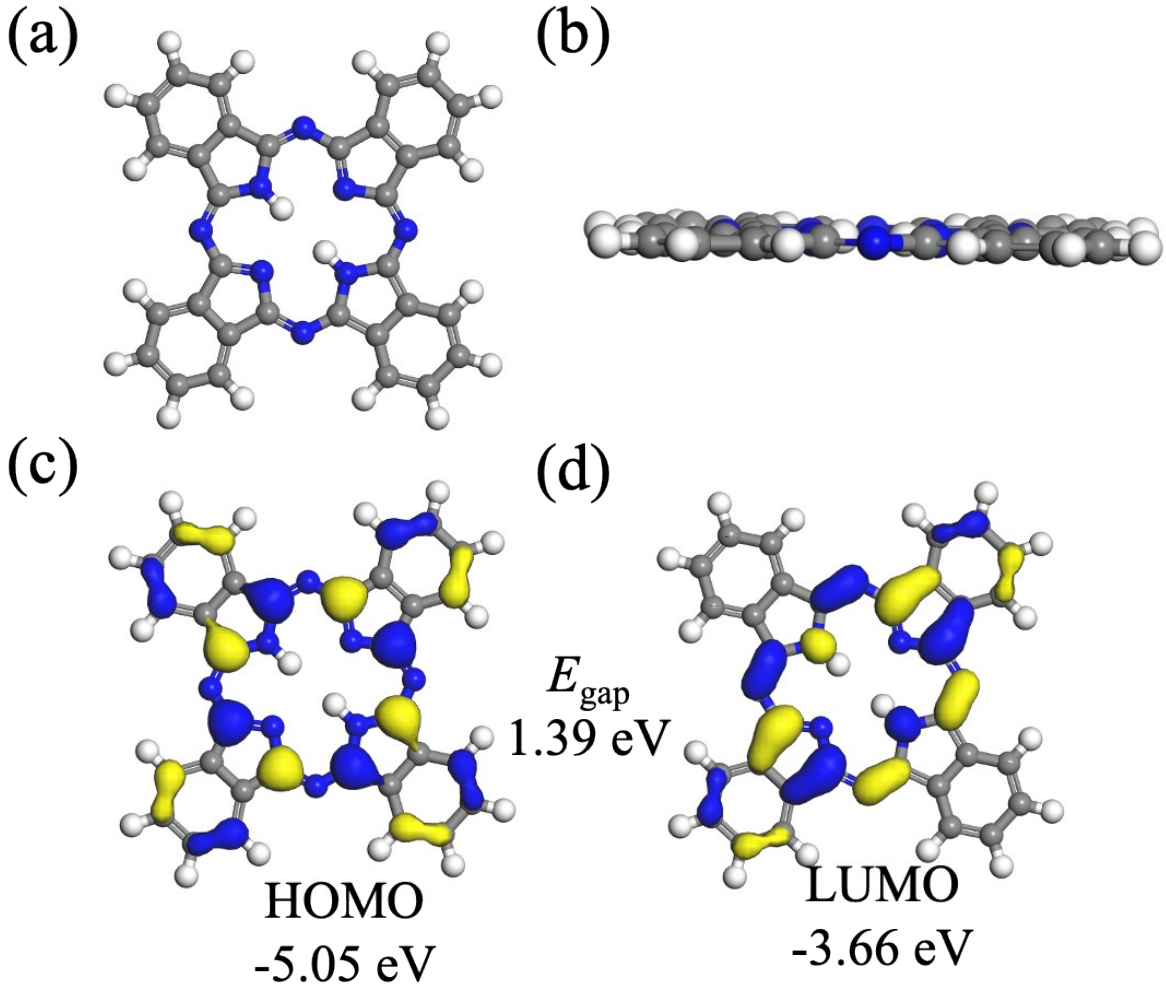

Figure S1. Optimized geometry of bare phthalocyanine (a, b), HOMO and LUMO plot of phthalocyanine (c, d)

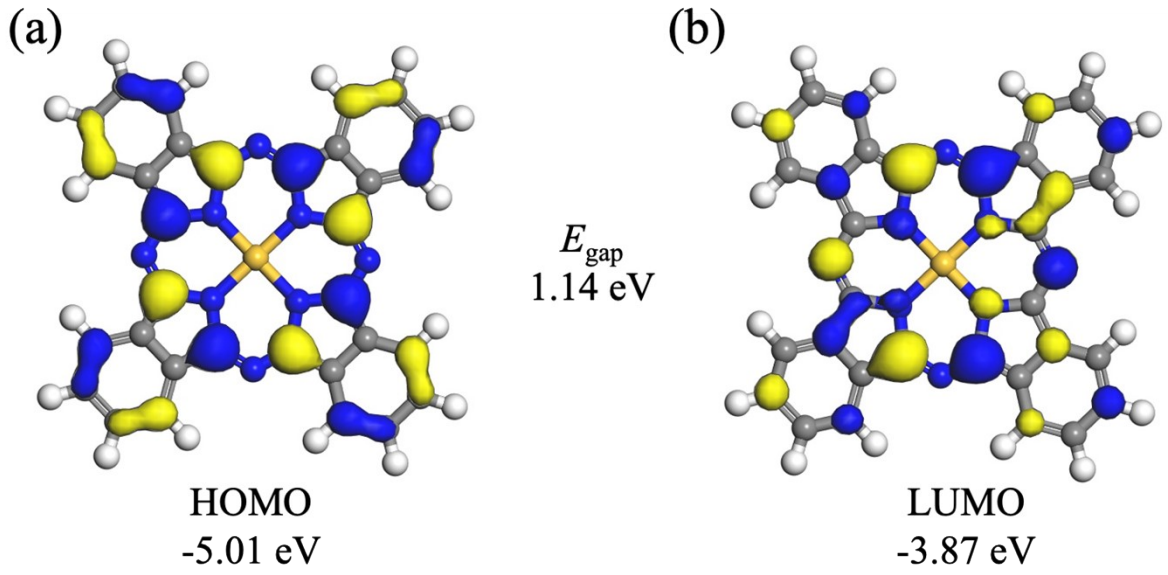

Figure S2. HOMO and LUMO plot of Si-decorated phthalocyanine (a, b)

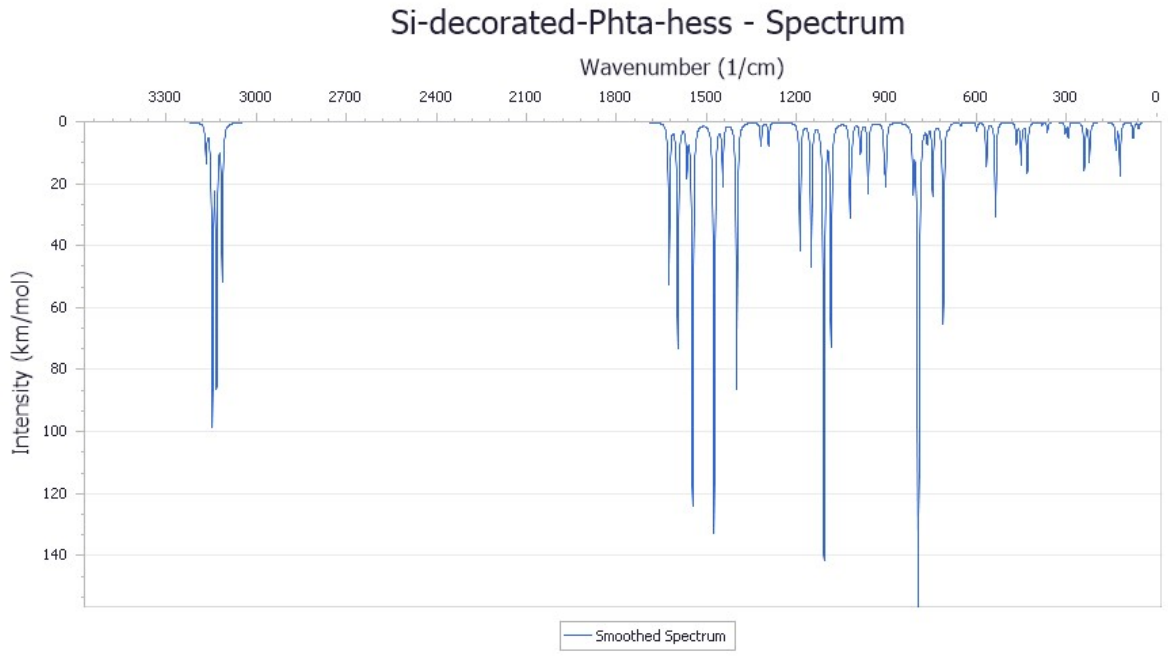

Figure S3. Vibrational spectrum of Si-decorated phthalocyanine

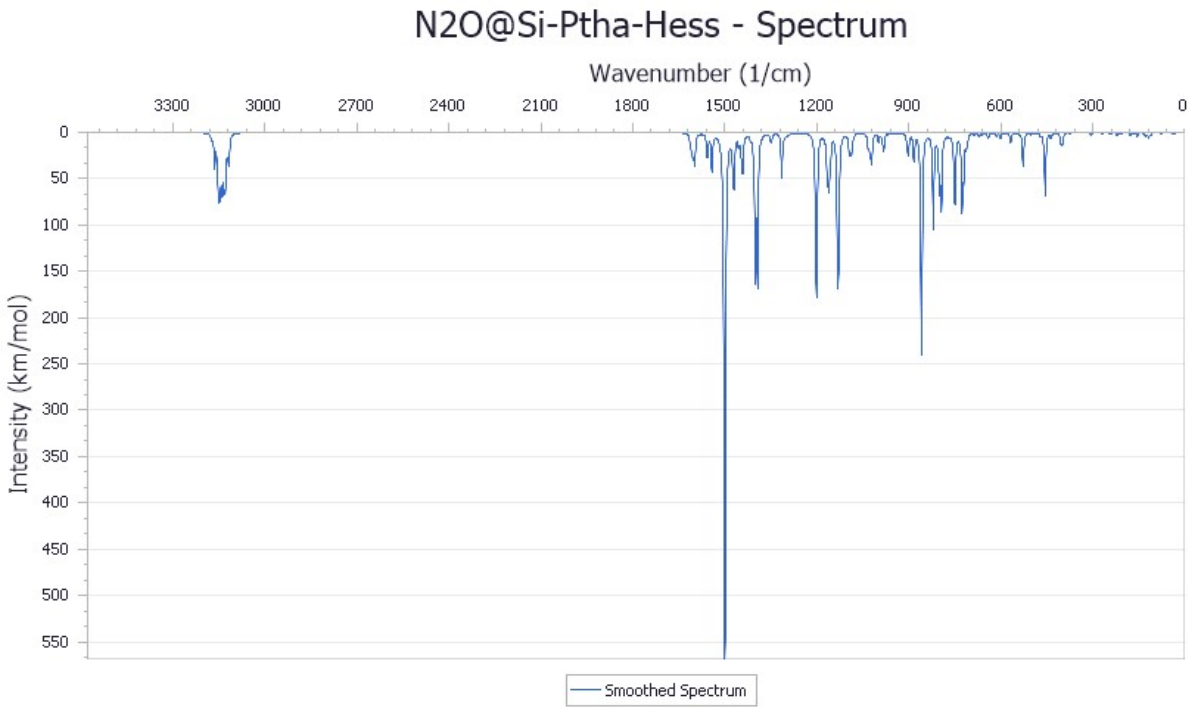

Figure S4. Vibrational spectrum of N_2O-N adsorption over Si-decorated phthalocyanine

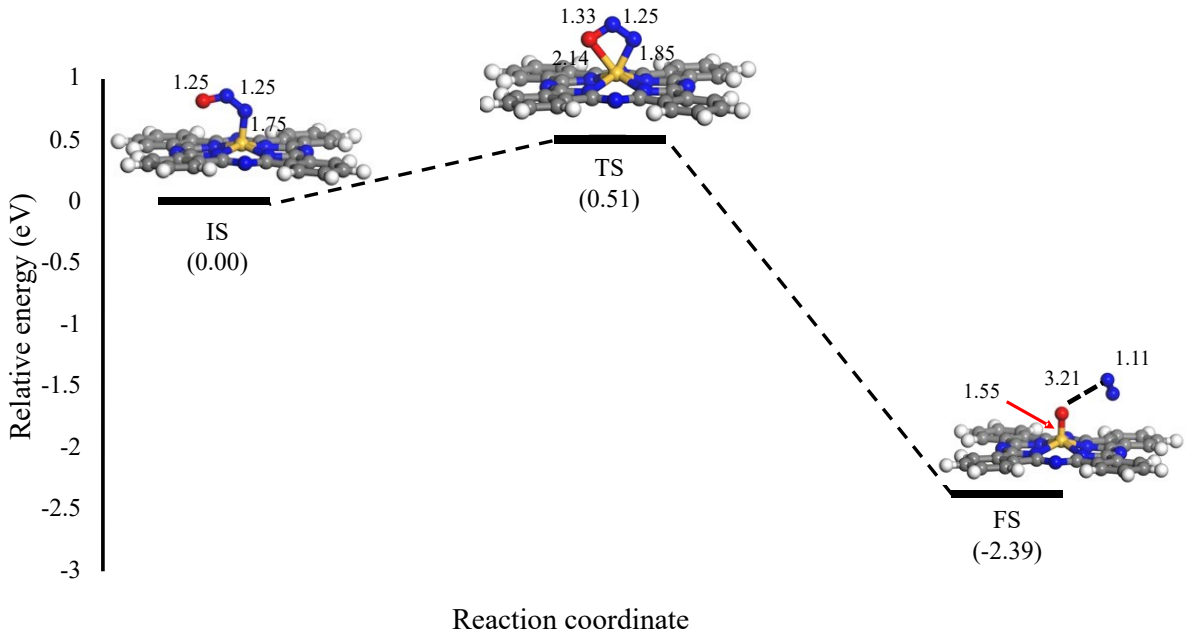

Figure S5. Relaxed stationary points for $N_2O \rightarrow N_2 + O^*$ reaction onto the Si@PathC catalyst. All bond distances are in Å

To further confirm the N_2O chemisorption of N_2O over the catalyst surface from its N-end we computed again the N_2O adsorption over the surface. This time N_2O is placed at little different position the geometry relaxation shows that the N_2O again chemisobred (as shown in IS in

Figure S5) with adsorption energy value of -1.14 eV, this time the N_2O molecule bent in upward position compared to N_2O adsorption from N-end mentioned in the main manuscript.

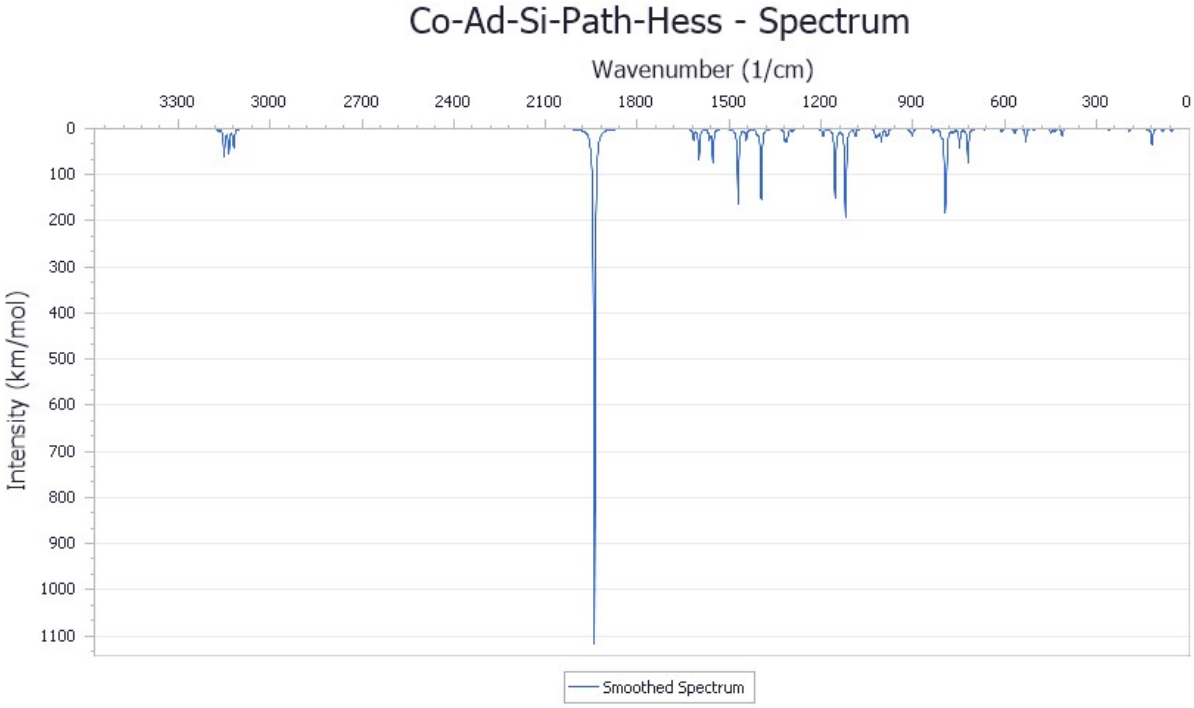

Figure S6. Vibrational spectrum of CO adsorption over Si-decorated phthalocyanine

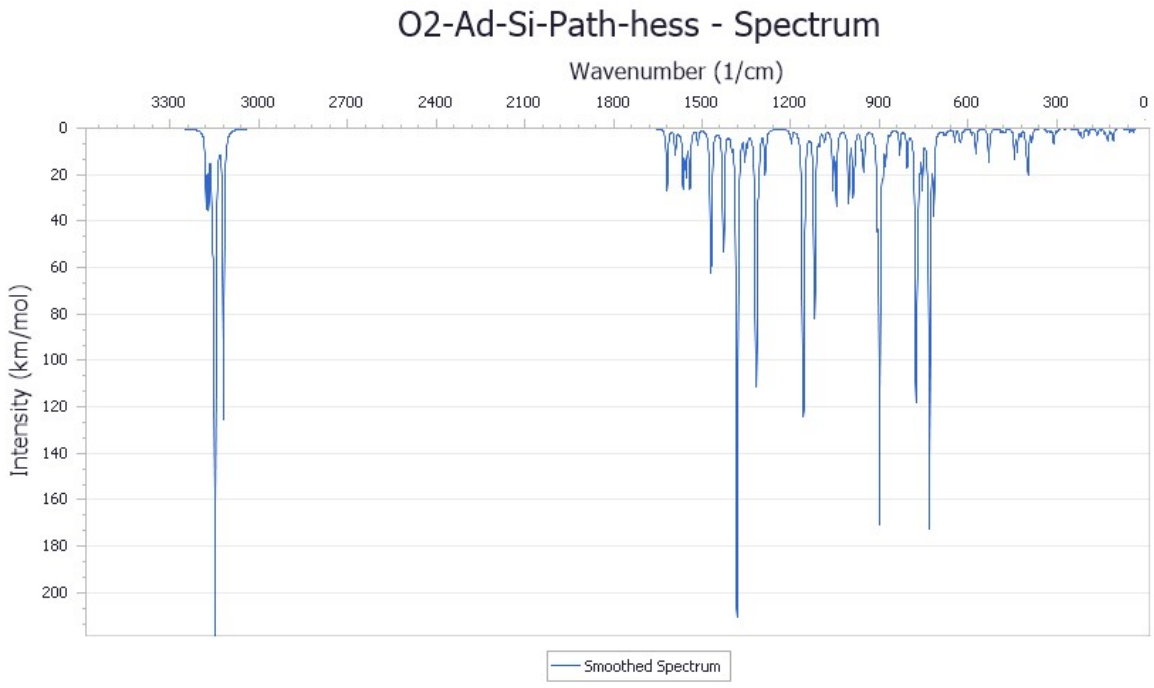

Figure S7. Vibrational spectrum of O_2 adsorption over Si-decorated phthalocyanine