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# Supporting Information

## Transition metal decorated phthalocyanine as potential host material for lithium polysulfides: a first-principles study

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Table S1. The formation energy ($E_f$) of all optimized TMPc structures.

| **TMPc** | $E_f$ **(eV)** |
|---|---|
| YPc | -5.8239 |
| ZrPc | -4.4653 |
| NbPc | -2.9180 |
| MoPc | -2.5938 |
| TcPc | -2.6510 |
| RuPc | -2.6136 |
| RhPc | -3.5866 |
| PdPc | -4.2735 |
| AgPc | 3.5829 |
| CdPc | -2.6117 |

Table S2. Bond lengths in pristine $Li_2S$ cluster and TMPc-$Li_2S$ system.

| **Species** | $E_b$ **(eV)** | **$Li_1$-S Bond Length (Å)** | **$Li_2$-S Bond Length (Å)** | **M-S Bond Length (Å)** |
|---|---|---|---|---|
| Pristine $Li_2S$ | / | 2.09 | 2.09 | / |
| $H_2Pc$ | 1.43 | 2.19 | 2.19 | / |
| YPc | 2.22 | 2.28 | 2.28 | 2.62 |
| ZrPc | 5.18 | 2.40 | 2.41 | 2.42 |
| NbPc | 4.63 | 2.36 | 2.37 | 2.33 |
| MoPc | 3.11 | 2.33 | 2.28 | 2.31 |
| TcPc | 2.64 | 2.29 | 2.24 | 2.29 |
| RuPc | 3.65 | 2.21 | 2.24 | 2.35 |
| RhPc | 2.34 | 2.19 | 2.22 | 2.56 |
| PdPc | 0.86 | 2.19 | 2.19 | 3.77 |
| AgPc | 1.38 | 2.19 | 2.19 | 3.33 |
| CdPc | 3.35 | 2.24 | 2.23 | 2.45 |

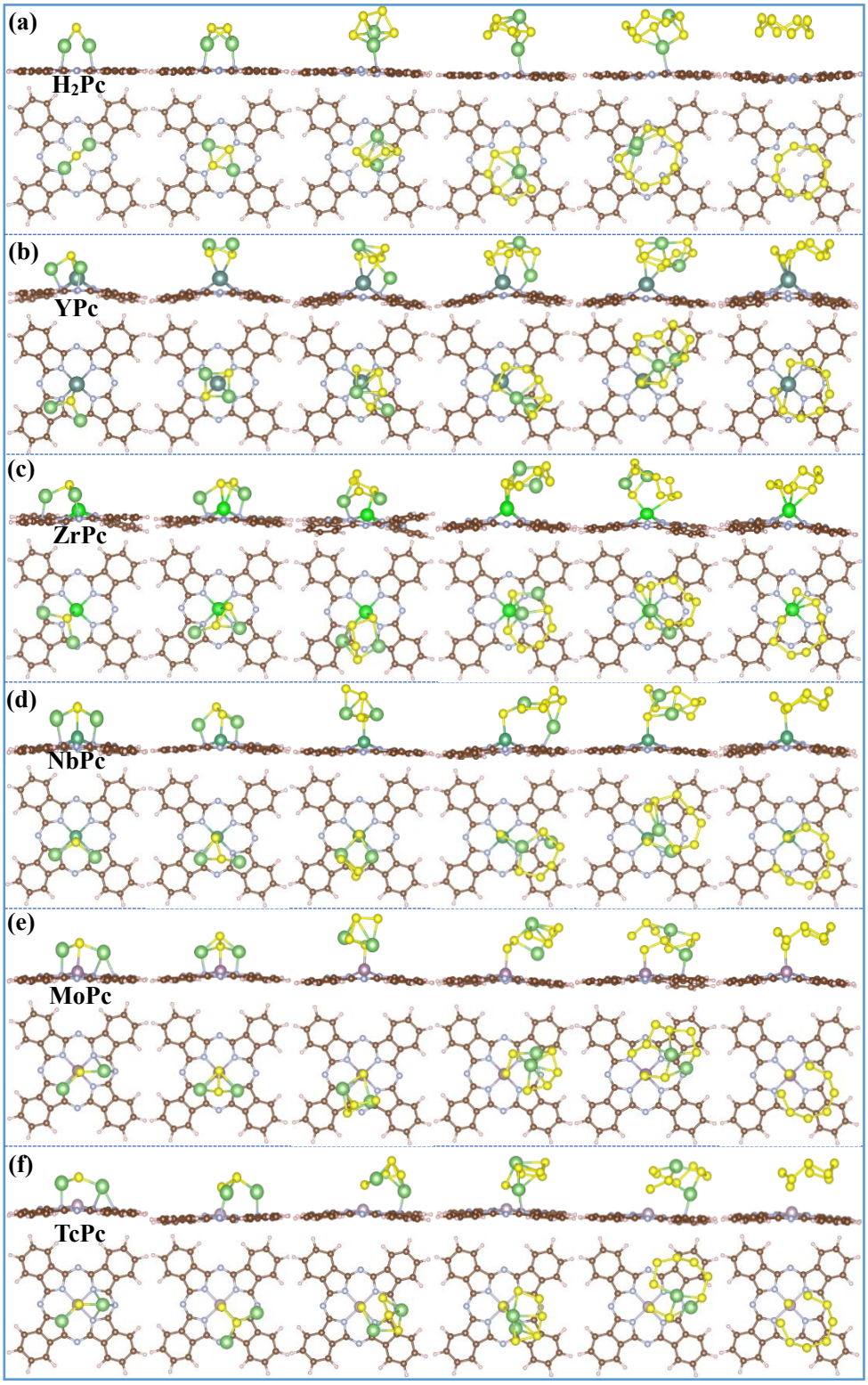


Fig. S1. (a)-(f) are the fully relaxed lowest-energy binding configurations of $S_8/Li_2S_x$ ($x$ = 1, 2, 4, 6, 8) adsorbed on $H_2Pc$/TMPc (TM = Y, Zr, Nb, Mo, Tc) substrates. Here, the top view and side view are given, respectively.

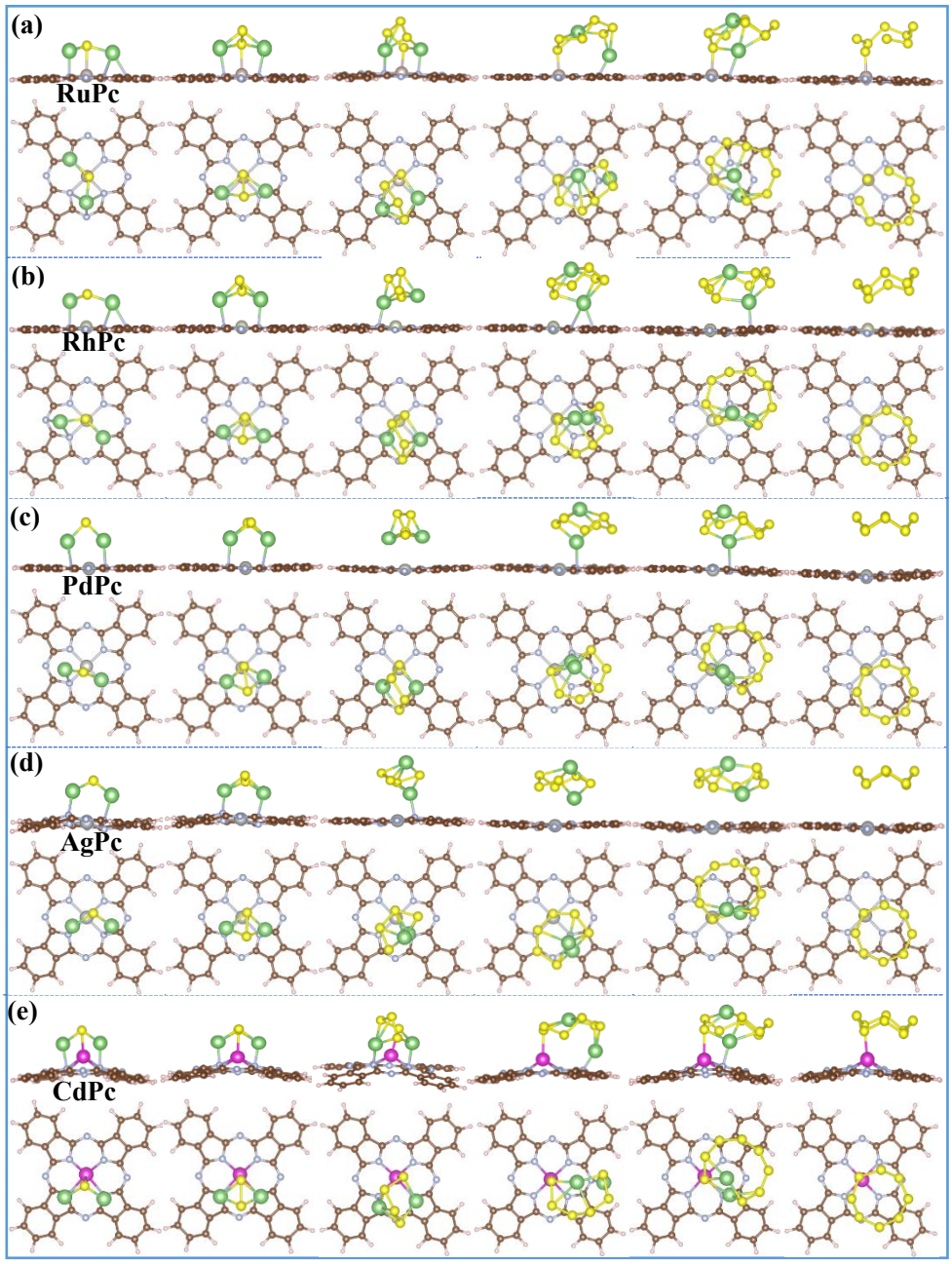


Fig. S2. (a)-(e) are the fully relaxed lowest-energy binding configurations of $S_8/Li_2S_x$ ($x$ = 1, 2, 4, 6, 8) adsorbed on $H_2Pc$/TMPc (TM = Tc, Ru, Pd, Ag, Cd) substrates. Here, the top view and side view are given, respectively.

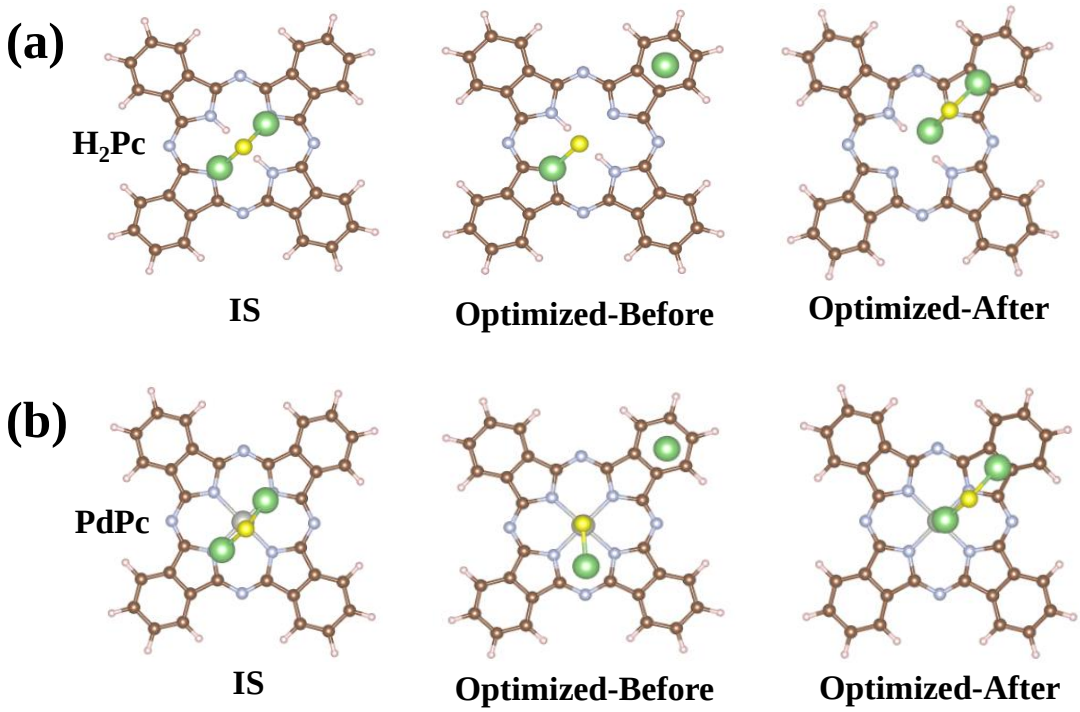


Fig. S3. The stable structures (IS), decomposed $Li_2S$ adsorption structures before and after optimization of the (a) $H_2Pc$-$Li_2S$ and (b) PdPc-$Li_2S$ systems.

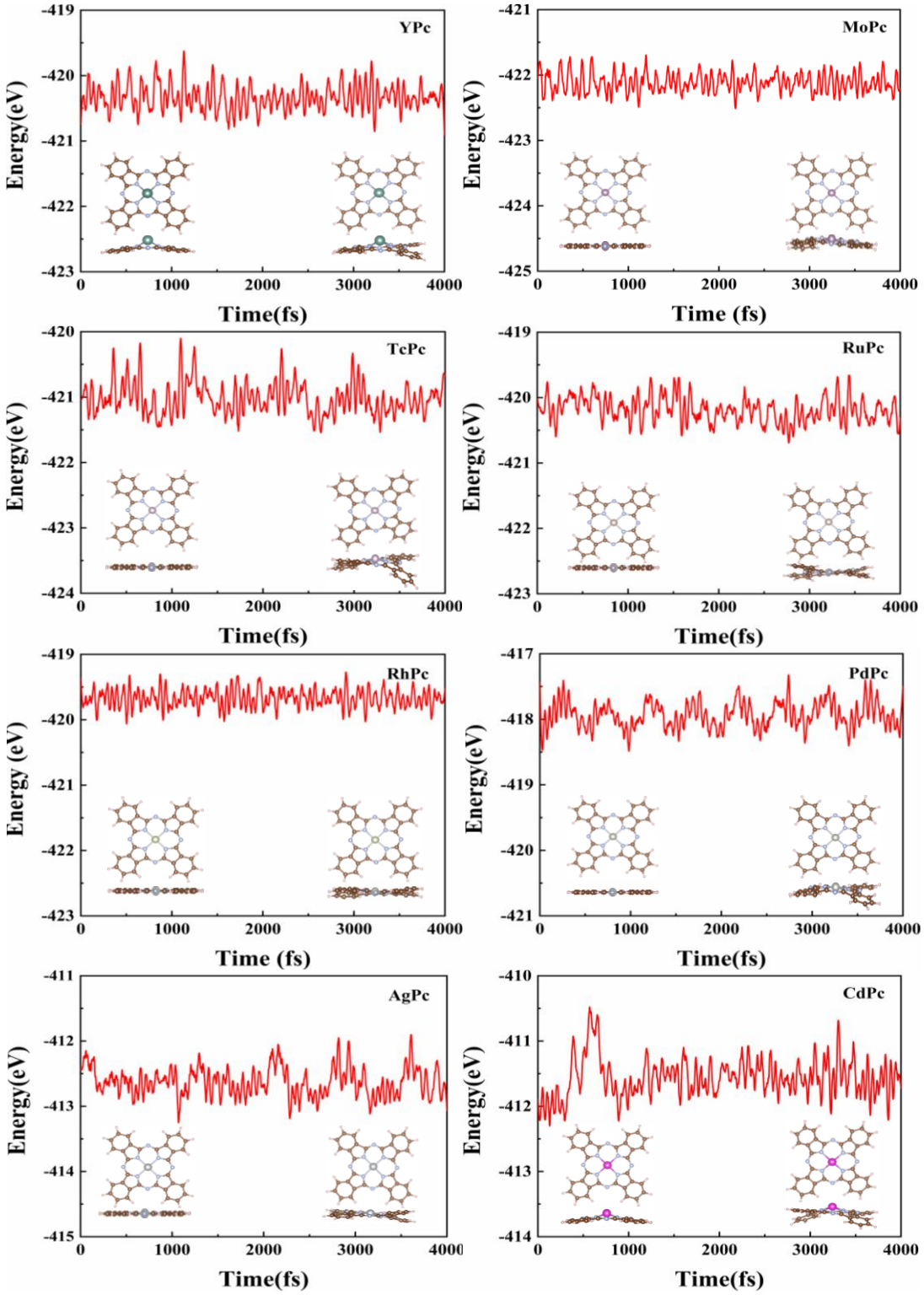


Fig. S4. The results of AIMD simulation of (Y、Mo、Tc、Ru、Rh、Pd、Ag and Cd)Pc structures, respectively. The illustration in the lower left corner is the optimized TMPc(TM= Y、Mo、Tc、Ru、Rh、Pd、Ag and Cd) structures, and the lower right corner is after AIMD simulation.