Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Phosphomolybdic Acid Supported Atomically Dispersed Transition Metal Atoms (M = Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au): Stable Single Atom Catalysts Studied by Density Functional Theory

Shujiao Wang,[a] Yingxin Feng,[a] Sen Lin,*,[a] and Hua Guo[b]

[a]*State Key Laboratory of Photocatalysis on Energy and Environment, College of Chemistry, Fuzhou University, Fuzhou 350002, People's Republic of China.*

[b]*Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131, USA.*

E-mail: slin@fzu.edu.cn (S. Lin)

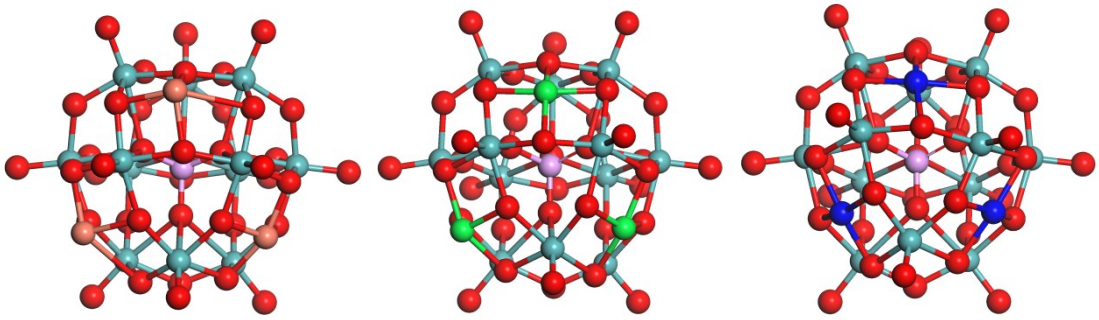

**Figure S1** Optimized configurations of M-PMA (M= Cu, Ru and Pt) with the numbers of M equal to 1, 2 and 3 at the 4-H site of PMA.

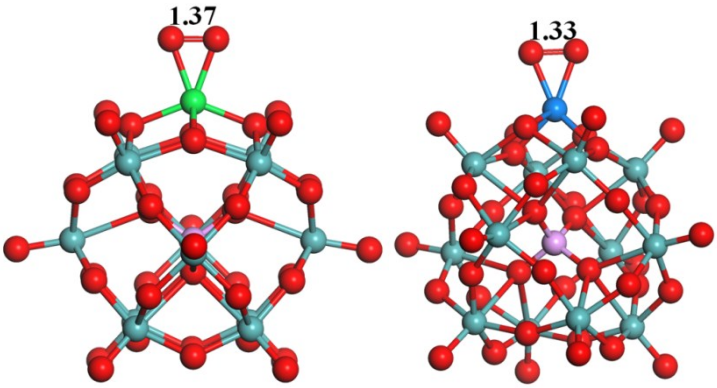


**Figure S2** Optimized configurations of an $O_2$ molecule adsorbed on M-PMA (M= Ru and Fe).

**Table S1** Calculated adsorption energies ($E_{ads}$/eV) for M (M= Cu, Ru and Pt) on PMA with M initially positioned at 4-H, 3H-$O_c$, 3H-$O_{bri}$, and B-$O_c$-$O_{bri}$, respectively.

| $M_1$ | Initial position | $E_{ads}$(eV) after optimization |
|---|---|---|
| Cu | 4-H | -7.50 |
| | 3H-$O_c$ | -7.50 |
| | 3H-$O_{bri}$ | -5.02 |
| | B-$O_c$-$O_{bri}$ | -4.49 |
| Ru | 4-H | -11.04 |
| | 3H-$O_c$ | -11.10 |
| | 3H-$O_{bri}$ | -9.70 |
| | B-$O_c$-$O_{bri}$ | -9.66 |
| Pt | 4-H | -7.92 |
| | 3H-$O_c$ | -5.95 |
| | 3H-$O_{bri}$ | -5.95 |
| | B-$O_c$-$O_{bri}$ | -5.21 |

**Table S2** Calculated adsorption energies (eV) of M (Pt, Ru and Cu) on PMA at the 4-H site with the numbers of M equal to 1, 2 and 3.

| M-PMA | Numbers of M | $E_{ads}$ |
|---|---|---|
| Pt | 1 | -7.92 |
| | 2 | -6.14 |
| | 3 | -5.23 |
| Ru | 1 | -11.69 |
| | 2 | -9.49 |
| | 3 | -8.56 |
| Cu | 1 | -7.23 |
| | 2 | -5.11 |
| | 3 | -4.36 |

**Table S3** The comparison between $E_{ad}$ values (eV) and the experimental metal cohesive energies ($E_{coh}$)

| M | $E_{ads}$ | $E_{coh}$ |
|---|---|---|
| Group VIII | | |
| Fe | -10.90 | -4.28 |
| Ru | -11.04 | -6.74 |
| Os | -11.24 | -8.17 |
| Group IX | | |
| Co | -10.41 | -4.39 |
| Rh | -9.11 | -5.74 |
| Ir | -10.08 | -6.94 |
| Group X | | |
| Ni | -9.35 | -4.44 |
| Pd | -6.44 | -3.90 |
| Pt | -7.92 | -5.85 |
| Group XI | | |
| Cu | -7.50 | -3.48 |
| Ag | -4.63 | -2.94 |
| Au | -5.04 | -3.81 |