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Keggin 型多酸负载的单原子催化剂(M_1/POM, M = Ni, Pd, Pt, Cu, Ag, Au, POM = $[PW_{12}O_{40}]^{3-}$)活化氮气分子的密度泛函理论计算研究

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DFT Study of POM-Supported Single Atom Catalyst (M_1/POM, M = Ni, Pd, Pt, Cu, Ag, Au, POM = $[PW_{12}O_{40}]^{3-}$) for Activation of Nitrogen Molecules

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表 S1　密度泛函理论计算出的所有 Pt_1/POM 各种自旋态的总能量

Table S1　DFT-derived total energy including electronic and zero-point energies of all POM complexes with different spin states.

Polyoxometalates	Spin multiplicity	Total energy/(a.u.)	Total energy/(kJ·mol^{-1})
Ni-POM	1	−4336.179957	−12201064.42
	3	−4336.183498	−12201074.38
Pd-POM	1	−4285.928488	−12059667.75
	3	−4293.579266	−12081195.37
Pt-POM	1	−4285.928488	−12059667.75
	3	−4285.924644	−12059656.93
Cu-POM	2	−4472.568778	−12584832.81
Ag-POM	2	−4422.179353	−12443047.96
Au-POM	2	−4411.808795	−12413867.47

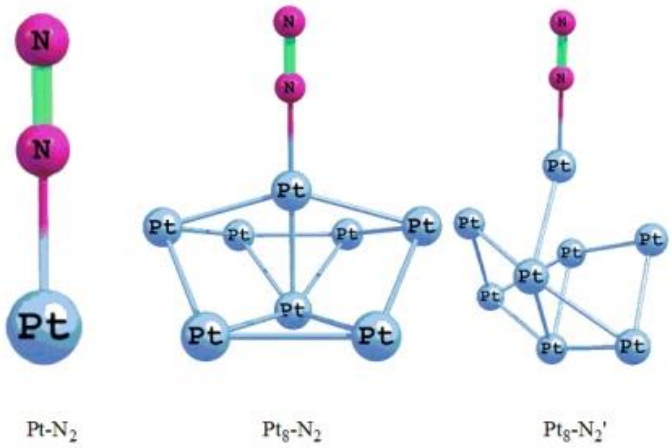

图 S1　独立金属 Pt 原子及 8 个 Pt 原子团簇吸附 N_2 后的模型

Fig.S1　The model of adsorption of N2 by independent Pt atom and 8 Pt atom clusters.

表S2　独立金属Pt原子及8个Pt原子团簇吸附N_2后的几何参数与Pt-POM的对比

Table S2　Comparison of geometric parameters and Pt-POM after adsorption of N_2 by independent Pt and 8 Pt groups.

Parameter	Pt-POM	Pt-N_2	Pt_8-N_2	Pt_8-N_2'
N-N	1.1394	1.1308	1.1247	1.1295
WBI(N-N)	2.5282	2.6193	2.7153	2.6561
E_{ad}	−241.04	−212.13	−125.52	−171.54