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

The Single Metal Atom (Ni, Pd, Pt) Anchored on Defective Hexagonal Boron Nitride for Oxidative Desulfurization

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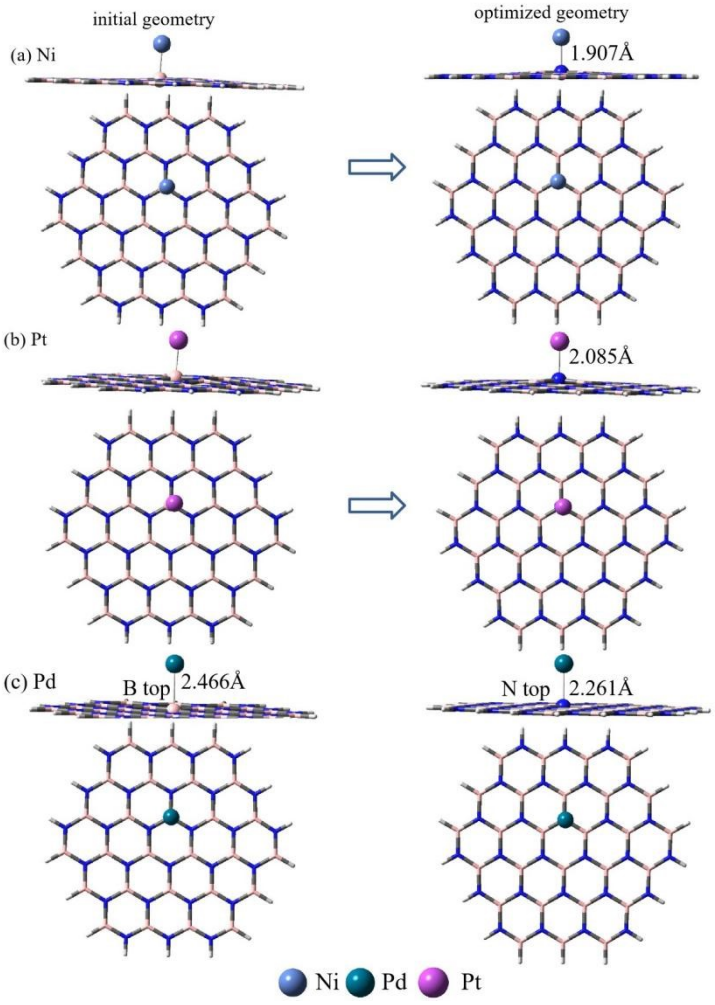

Fig.S1. The initial geometry and optimized geometry for (a) Pt and (b)Ni on the pristine h-BN

surface, (c) denotes Pd atom adsorption on top of B and N site.

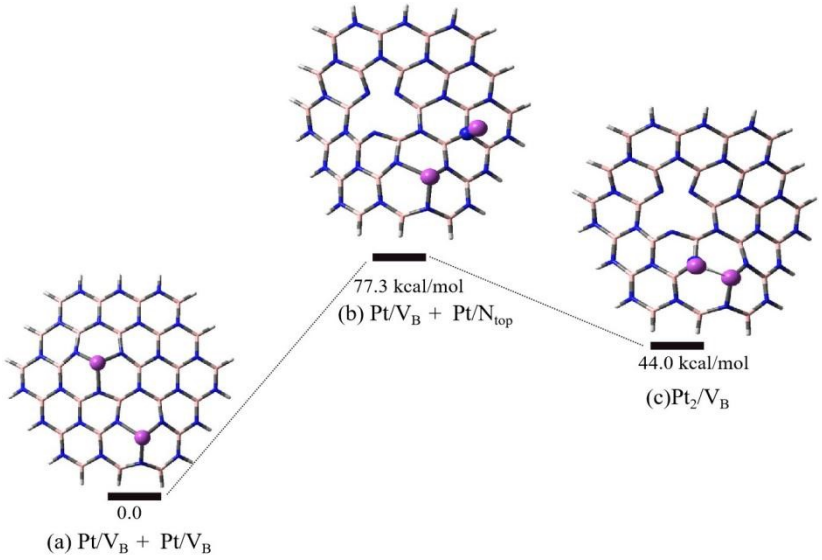

Fig. S2. Geometries and energies (kcal/mol) in the process of Pt dimerization.(a) denotes two Pt atoms anchored on the V_B sites, (b) denotes the intermediate in which one of the Pt atoms diffuses on the top of N atom, and (c) denotes the formation of the Pt dimer. The purple ball denotes the Pt atoms.

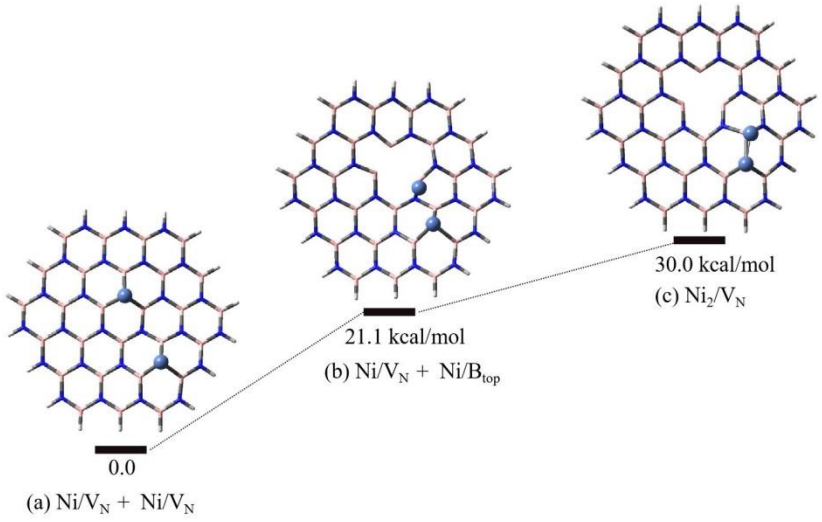

Fig. S3. Geometries and energies (kcal/mol) in the process of Ni dimerization.(a) denotes two Ni atoms anchored on the V_N sites, (b) denotes the intermediate in which one of the Ni atoms diffuses on the top of N atom, and (c) denotes the formation of the Ni dimer. The gray blue ball denotes Ni atoms.

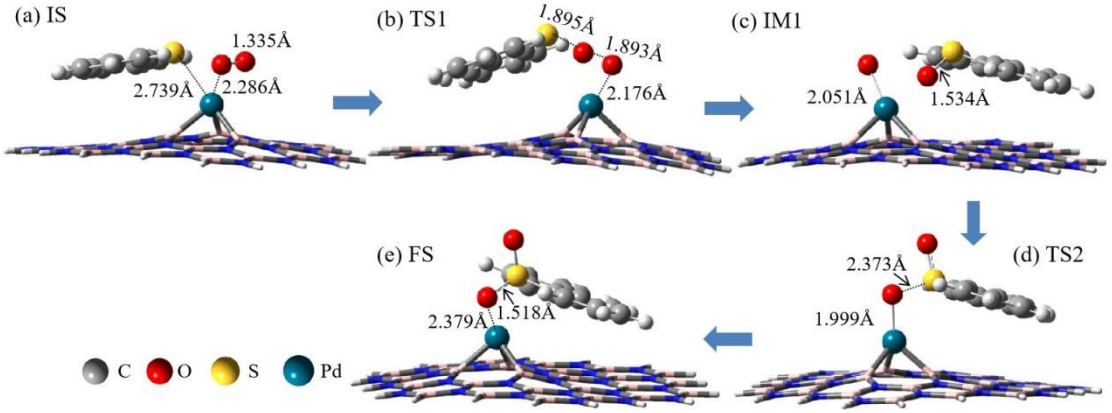

Figure S4. Geometries of initial states (ISs), transition states (TSs), intermediates (IMs), and final state (FSs) for DBT oxidation on Pd/V_N.

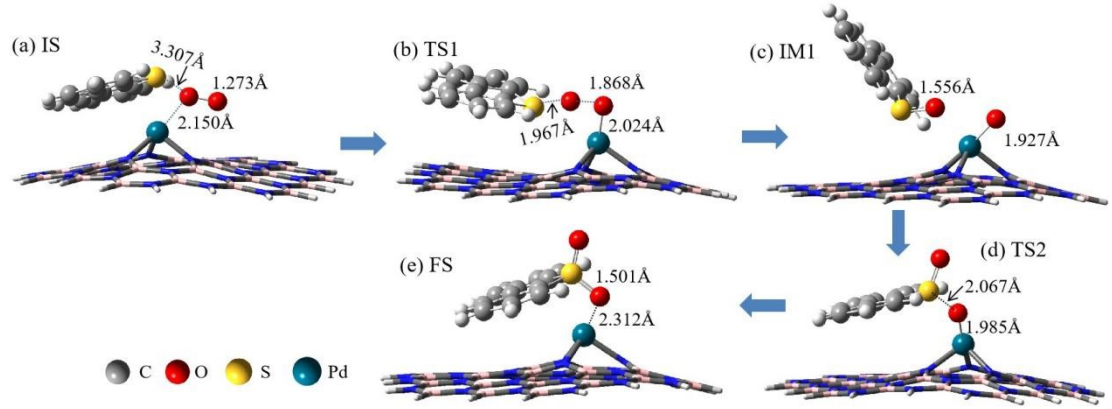

Figure S5. Geometries of initial states (ISs), transition states (TSs), intermediates (IMs), and final state (FSs) for DBT oxidation on Pd/V_B.

Table S1. The adsorption energy of O_2 on the M/V_B and M/V_N (unit: kcal/mol), O−O and M−O bond length (in Å), the NPA charge on O_2 and the doped M.

	M/V_B			M/V_N		
Properties	Ni/V_B	Pd/V_B	Pt/V_B	Ni/V_N	Pd/V_N	Pt/V_N
Eads (kcal/mol)	6.3	−3.1	−14.4	−37.6	−24.3	−25.0
O−O distance	1.297	1.298	1.313	1.339	1.337	1.339
M−O distance	1.973	2.172	2.180	1.973	2.205	2.195
Charge on O_2	−0.234	−0.291	−0.326	−0.432	−0.628	−0.495
Charge on M	0.736	0.849	1.021	−0.084	0.047	0.066

Table S2. The binding energy of M on V_B and V_N (unit: kcal/mol) in the previous references and this work.

	Ref		This work	
	V_B	V_N	V_B	V_N
Ni	−187.7(53)	−115.3(53)	−161.3	−107.1
	−184.7(45)	−112.1(45)		
Pd	−122.9(46)	−104.0(46)	−87.8	−75.0
	−120.8(50）			
Pt	−141.8(45)	−143.4(45)	−117.2	−129.7
	−150.6(50)			

Reference

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