

(a)

PBE lattice constant vs HSE  
lattice constant (color by pure,  
A-mixed, B-mixed, X-mixed)  
(JIAQI)

(b)

PBE decomp. energy vs PBE  
band gap (color by pure, A-  
mixed, B-mixed, X-mixed)  
(JIAQI)

(c)

PBE decomp. energy vs PV  
figure of merit (color by pure, A-  
mixed, B-mixed, X-mixed)  
(JIAQI)

(d)

HSE decomp. energy vs HSE  
band gap (color by pure, A-  
mixed, B-mixed, X-mixed)  
(JIAQI)