补充材料

二维 XO_2 $(X = \text{Ni, Pd, Pt})$ 弹性、电子结构和热导率*

方文玉 [1]# 陈粤 [1]# 叶盼 [1] 魏皓然 [1] 肖兴林 [1]

黎明锴 [1]† Ahuja Rajeev [2] 何云斌 [1]‡

1) (湖北大学材料科学与工程学院, 铁电压电材料与器件湖北省重点实验室, 高分子材料湖北省重点实验室,

功能材料绿色制备与应用教育部重点实验室, 武汉 430062)
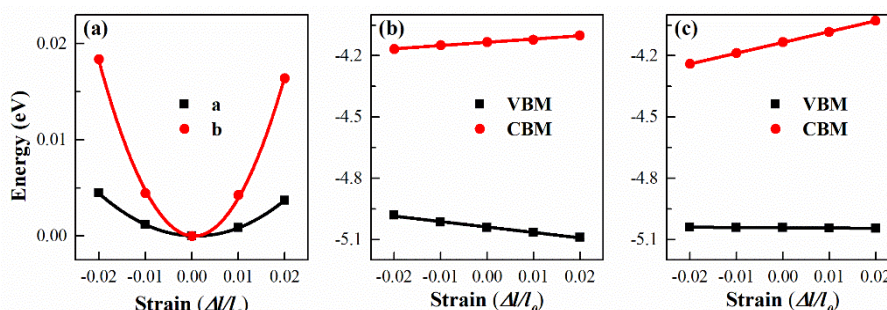2) (乌普萨拉大学物理与天文系凝聚态理论组, 瑞典乌普萨拉 S-751-20)

图 S1 二维黑磷烯的平面刚度和形变势拟合示意图 (a) 晶胞总能的增量在不同应变量下的二次曲线拟合；(b), (c) a 和 b 两个方向上 VBM 和 CBM 相对真空能级的位置，与应变量之间做线性拟合

Fig. S1. Schematic diagram of plane stiffness and deformation potential of monolayer phosphorene: (a) Quadratic fitting of the energy difference to the uniaxial strain are used to calculate the plane stiffness; (b) and (c) linear fitting of the energy of VBM and CBM relative to the uniaxial strain along a and b direction, which are used to calculate the deformation potential.

表 S1 二维 XO_2 和 BP 在不同应变下的真空能级

Table S1. Vacuum-level of monolayer XO_2 and BP at different strains.

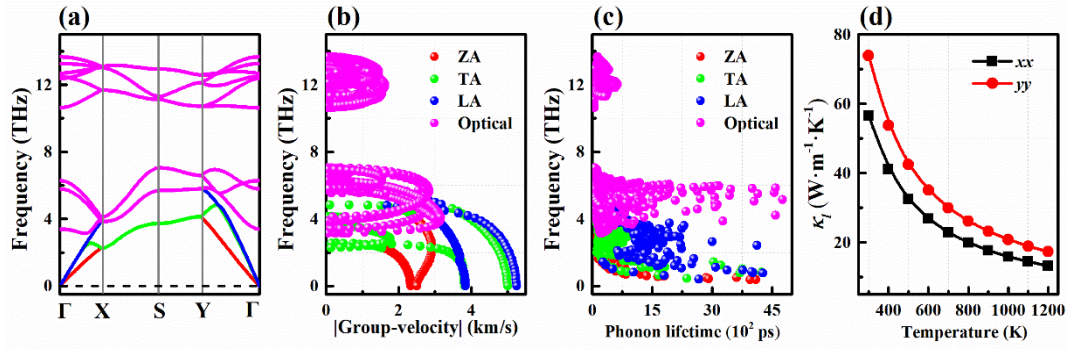| Monolayers	Along armchair/a direction /eV				host	Along zigzag/b direction /eV			
	-2%	-1%	1%	2%	0.0%	-2%	-1%	1%	2%
NiO_2	1.845	1.825	1.788	1.770	1.806	1.845	1.825	1.788	1.770
PdO_2	1.895	1.874	1.833	1.813	1.853	1.895	1.874	1.833	1.813
PtO_2	1.916	1.895	1.854	1.834	1.875	1.916	1.895	1.854	1.834
BP	2.764	2.810	2.787	2.741	2.720	2.810	2.787	2.741	2.719

图 S2 单层黑磷烯的(a)声子谱、(b) 群速度、(c) 声子寿命和(c) 晶格热导率

Fig. S2. (a) Phonon dispersion, (b) group velocity, (c) phonon lifetime and lattice thermal conductivity of Phosphorene