Supporting Information for *Acta Phys. -Chim. Sin.* doi: 10.3866/PKU.WHXB202007015

全无机卤化铅钙钛矿的结构、热力学稳定性和电子性质

李亚文[1]，那广仁[1]，罗树林[1]，贺欣[1,2,*]，张立军[1,*]

[1] 集成光电子学国家重点实验室，教育部汽车材料重点实验室，吉林大学材料科学与工程学院，长春 130012

[2] 吉林大学物理学院，长春 130012

Structural, Thermodynamical and Electronic Properties of All-Inorganic Lead Halide Perovskites

Yawen Li [1], Guangren Na [1], Shulin Luo [1], Xin He [1,2,*], Lijun Zhang [1,*]

[1] State Key Laboratory of Integrated Optoelectronics, Key Laboratory of Automobile Materials of MOE, College of Materials Science and Engineering, Jilin University, Changchun 130012, China.

[2] College of Physics, Jilin University, Changchun 130012, China.

[*]Corresponding authors. Emails: xin_he@jlu.edu.cn (X.H.); lijun_zhang@jlu.edu.cn (L.Z.).

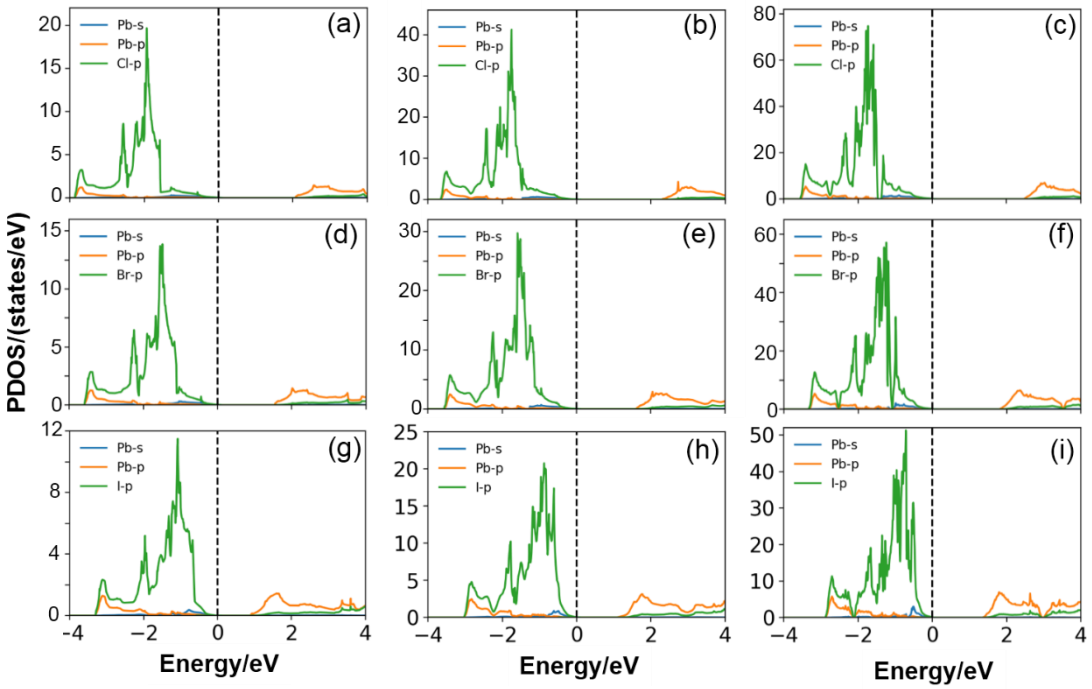

Fig. S1 The HSE + SOC functional project density of states (PDOS) of (a–c) α/β/γ-$CsPbCl_3$, (d–f) α/β/γ-$CsPbBr_3$ and (g–i) α/β/γ-$CsPbI_3$.

Table S1 HSE+SOC functional calculated effective masses of α/β/γ-phase $CsPbX_3$ (m_e^* and m_h^* for electron and hole, respectively).

	cubic	m^*	tetragonal		m^*	orthorhombic			m^*
	<100>		<100>	<001>		<100>	<010>	<001>	
$CsPbCl_3$									
m_e^*	0.1	0.1	0.132	0.113	0.134	0.164	0.115	0.173	0.146
m_h^*	0.115	0.115	0.148	0.119	0.127	0.164	0.115	0.151	0.14
$CsPbBr_3$									
m_e^*	0.081	0.081	0.097	0.084	0.092	0.131	0.106	0.138	0.123
m_h^*	0.078	0.078	0.097	0.084	0.092	0.131	0.132	0.138	0.134
$CsPbI_3$									
m_e^*	0.05	0.05	0.092	0.057	0.076	0.091	0.078	0.099	0.089
m_h^*	0.056	0.056	0.101	0.078	0.092	0.13	0.104	0.11	0.114

The transport effective masses m^* calculated by the formula: $1/m^* = 1/3(1/m_x + 1/m_y + 1/m_z)$.