

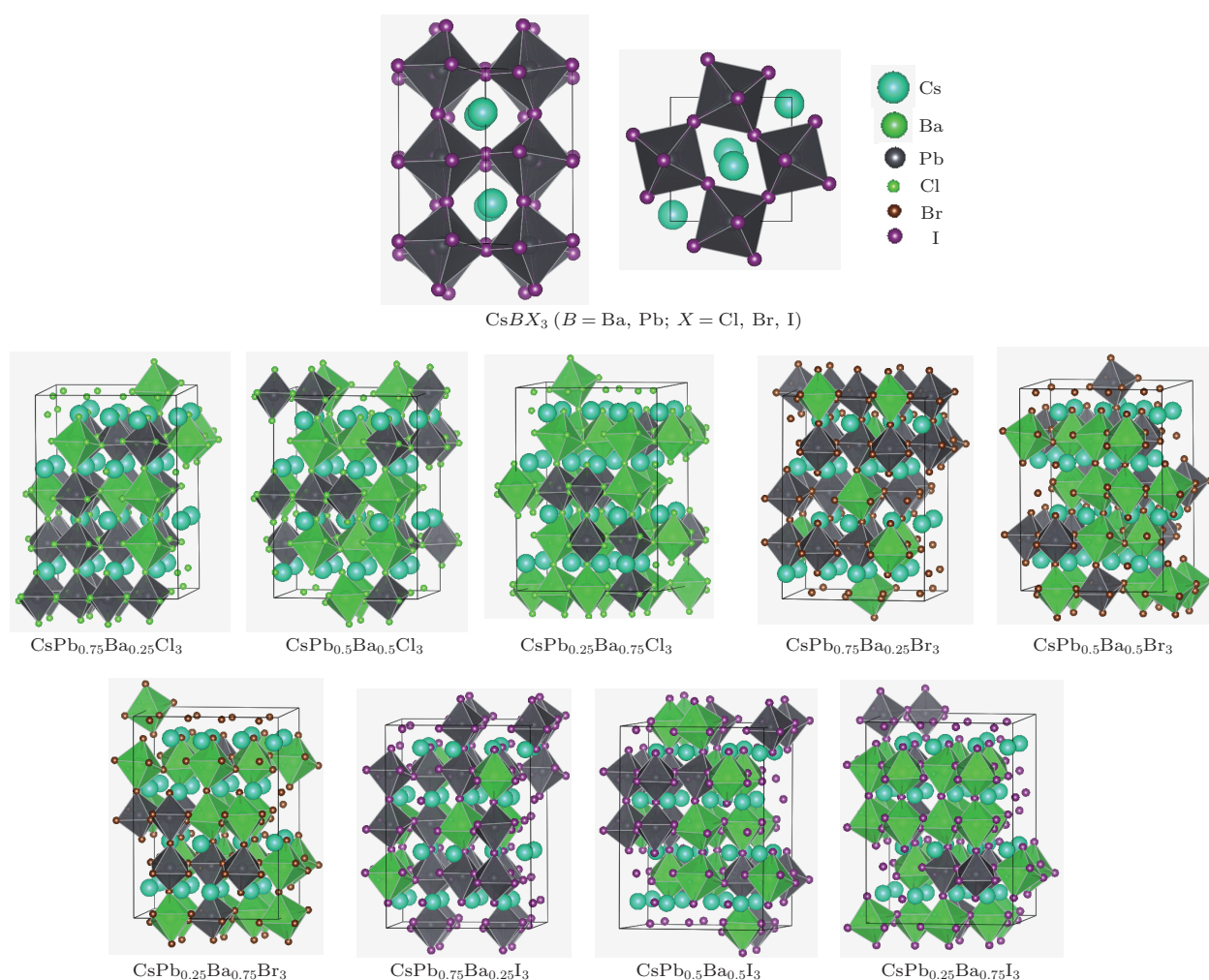
钡作为掺杂元素调控铅基钙钛矿材料的 毒性和光电特性*

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图S1和表S1分别给出了CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1)的晶体结构和晶胞参数.



图S1 CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1)的晶体结构

Fig. S1. Crystal structures of the alloyed perovskite CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1).

* 国家自然科学基金优秀青年基金 (批准号: 61722403) 资助的课题.

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表 S1 CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1) 的晶体结构信息

Table S1. Structural data of the alloyed perovskite CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1).

| | | <i>x</i> | | | | |
|---|--------------------------|----------|---------|---------|---------|---------|
| | | 0 | 0.25 | 0.5 | 0.75 | 1 |
| CsPb _{1-x} Ba _x Cl ₃ | <i>a</i> /Å | 7.993 | 8.066 | 8.216 | 8.319 | 8.216 |
| | <i>b</i> /Å | 11.365 | 11.526 | 11.555 | 11.630 | 11.894 |
| | <i>c</i> /Å | 7.953 | 7.994 | 8.03 | 8.089 | 8.306 |
| | α/(°) | 90 | 90.003 | 89.965 | 90.033 | 90 |
| | β/(°) | 90 | 90.013 | 90.044 | 90.028 | 90 |
| | γ/(°) | 90 | 89.977 | 90.045 | 89.994 | 90 |
| | <i>V</i> /Å ³ | 722.49 | 743.30 | 762.17 | 782.70 | 811.73 |
| CsPb _{1-x} Ba _x Br ₃ | <i>a</i> /Å | 8.388 | 8.546 | 8.740 | 8.854 | 8.820 |
| | <i>b</i> /Å | 11.978 | 12.056 | 12.148 | 12.245 | 12.480 |
| | <i>c</i> /Å | 8.353 | 8.334 | 8.359 | 8.443 | 8.691 |
| | α/(°) | 90 | 89.999 | 89.969 | 90.073 | 90 |
| | β/(°) | 90 | 89.997 | 89.965 | 90.047 | 90 |
| | γ/(°) | 90 | 89.973 | 90.032 | 89.988 | 90 |
| | <i>V</i> /Å ³ | 839.34 | 858.60 | 887.54 | 915.36 | 956.59 |
| CsPb _{1-x} Ba _x I ₃ | <i>a</i> /Å | 9.021 | 9.206 | 9.362 | 9.493 | 9.527 |
| | <i>b</i> /Å | 12.768 | 12.812 | 12.888 | 13.004 | 13.349 |
| | <i>c</i> /Å | 8.760 | 8.778 | 8.862 | 8.938 | 9.068 |
| | α/(°) | 90 | 89.948 | 89.976 | 89.897 | 90 |
| | β/(°) | 90 | 89.914 | 89.973 | 89.970 | 90 |
| | γ/(°) | 90 | 90.061 | 89.983 | 89.999 | 90 |
| | <i>V</i> /Å ³ | 1008.99 | 1035.42 | 1069.35 | 1103.38 | 1153.37 |

结合能的计算公式如下:

$$\Delta E(x) = E(\text{CsPb}_{1-x}\text{Ba}_x\text{X}_3) - E(\text{Cs}) - (1-x)E(\text{Pb}) - xE(\text{Ba}) - 3E(\text{X}), \quad X = \text{Cl, Br, I}, \quad (1)$$

其中, $E(\text{CsPb}_{1-x}\text{Ba}_x\text{X}_3)$ 表示的 CsPb_{1-x}Ba_xX₃ 能量; $E(\text{Cs})$, $E(\text{Pb})$, $E(\text{Ba})$, $E(\text{X})$ 分别为自由原子 Cs, Pb, Ba, X 的能量. 化合物的结合能越低, 结构越稳定. 计算结果如图 S2 所示.

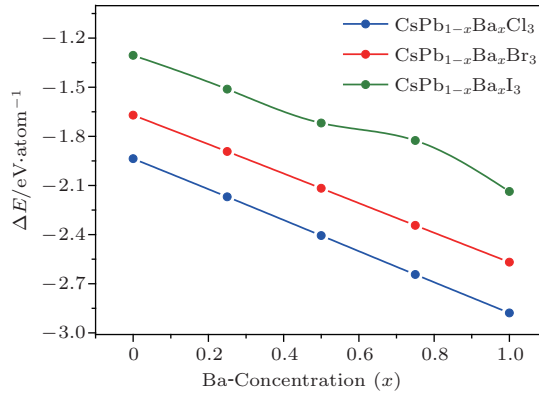


图 S2 计算得到的 CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1) 合金钙钛矿体系的结合能

Fig. S2. DFT-calculated binding energies of the alloyed perovskite CsPb_{1-x}Ba_xX₃ (X = Cl, Br, I; x = 0, 0.25, 0.5, 0.75, 1).

图 S3 和图 S4 分别给出了 CsPb_{1-x}Ba_xCl₃ 和 CsPb_{1-x}Ba_xBr₃ (x = 0, 0.25, 0.5, 0.75, 1) 合金钙钛矿体系的投影态密度.

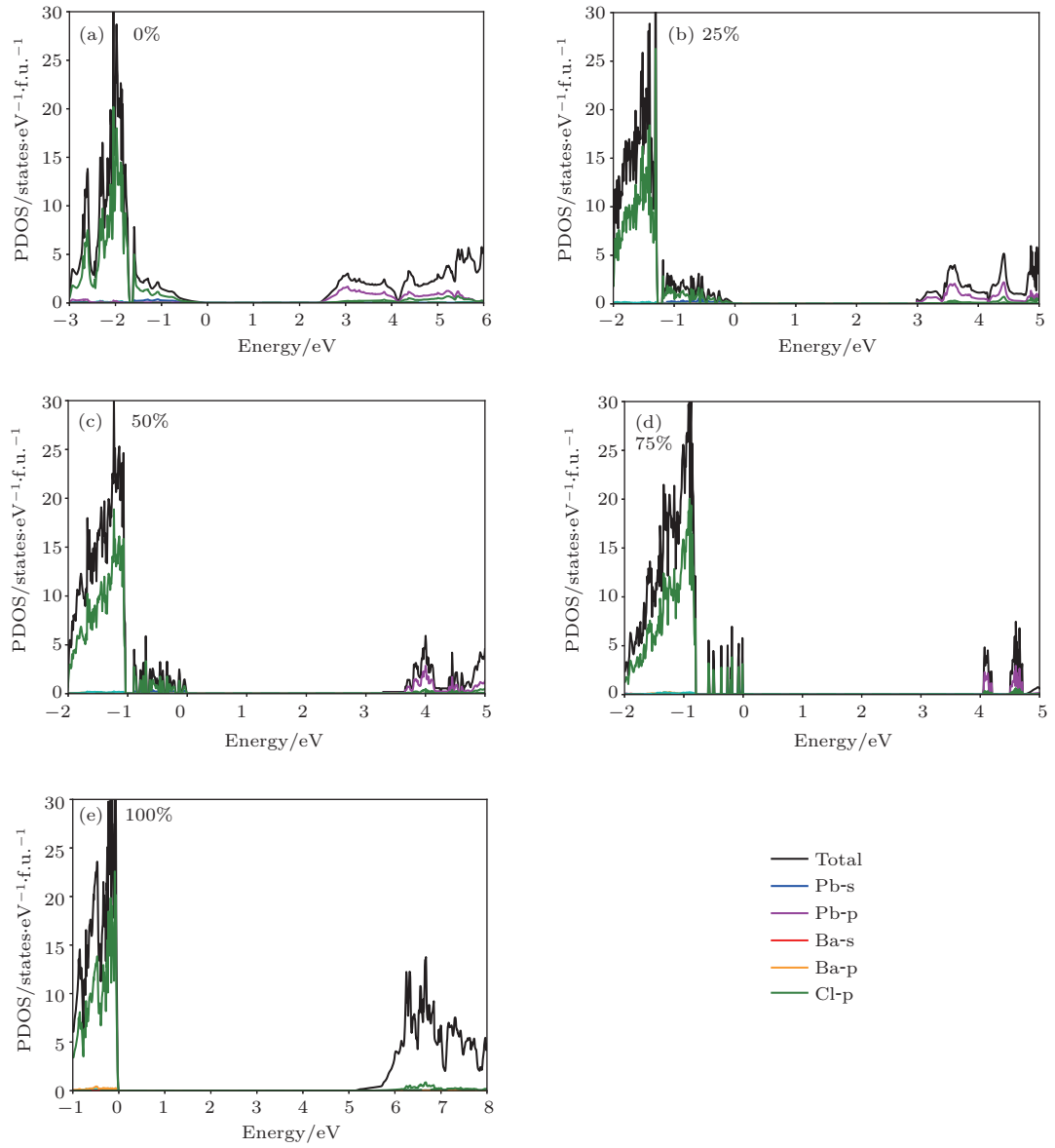
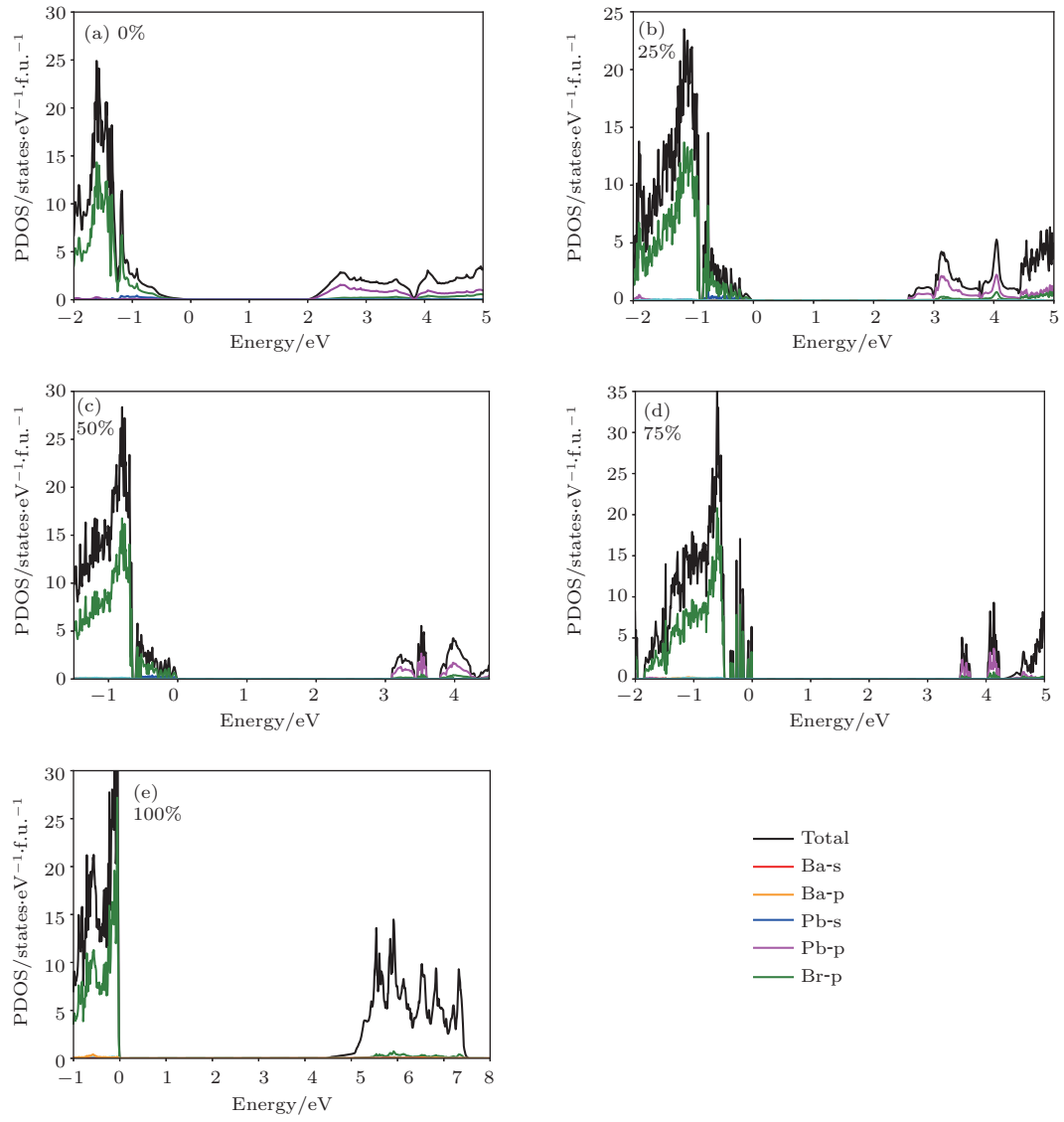


图 S3 计算得到的 $\text{CsPb}_{1-x}\text{Ba}_x\text{Cl}_3$ 合金钙钛矿体系的投影态密度 (a) $x = 0\%$; (b) $x = 25\%$; (c) $x = 50\%$; (d) $x = 75\%$; (e) $x = 100\%$

Fig. S3. Calculated atomic-orbital-projected density of states (PDOS) of the alloyed perovskite $\text{CsPb}_{1-x}\text{Ba}_x\text{Cl}_3$: (a) $x = 0\%$; (b) $x = 25\%$; (c) $x = 50\%$; (d) $x = 75\%$; (e) $x = 100\%$.



图S4 计算得到的 $\text{CsPb}_{1-x}\text{Ba}_x\text{Br}_3$ 合金钙钛矿体系的投影态密度 (a) $x = 0\%$; (b) $x = 25\%$; (c) $x = 50\%$; (d) $x = 75\%$; (e) $x = 100\%$

Fig. S4. Calculated atomic-orbital-projected density of states (PDOS) of the alloyed perovskite $\text{CsPb}_{1-x}\text{Ba}_x\text{Br}_3$: (a) $x = 0\%$; (b) $x = 25\%$; (c) $x = 50\%$; (d) $x = 75\%$; (e) $x = 100\%$.