

**Supporting information:**

**Structural, electronic, and optical properties of cubic formamidinium lead iodide perovskite: A first-principles investigation**

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The POSCAR file for FAPbI<sub>3</sub> PBE [111].

FAPbI<sub>3</sub> PBE [111]

```
1.0000000000000000
  6.4589972925718193    0.0000000000000000    0.0000000000000000
  0.0000000000000000    6.4589972925718193    0.0000000000000000
  0.0000000000000000    0.0000000000000000    6.4589972925718193
```

```
C    N    H    Pb    I
  1    2    5    1    3
```

Direct

```
0.4446100039999976  0.4784399710000002  0.5249500150000017
0.4421560795451001  0.6094450370013220  0.3706999280163501
0.5863716296305626  0.4718834382313304  0.6686733616323792
0.3189267628053969  0.3661898113936886  0.5342151560554598
0.3247655868173496  0.6012420605569488  0.2649740724251757
0.5524830491180950  0.7206484476027484  0.3514892894933936
0.7094075923344363  0.5702758137779185  0.6715301513277225
0.5768870461671369  0.3618426087835545  0.7817959997122372
0.0000000000000000  0.0000000000000000  0.0000000000000000
0.4955008036196986  0.0340738133587379  0.0084927291793448
0.0104307130704626  0.5068825151667298  0.0309936222465907
0.9559045289805326  0.9716826665041225  0.5159527464927507
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