Supplementary Information

Reply to "Comments on Density functional theory analysis of structural and electronic properties of orthorhombic perovskite $CH_3NH_3PbI_3$" by J. Even et al.

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The atomic Coordinates of orthorhombic perovskite $CH_3NH_3PbI_3$ materials.

Pb	4.416348	12.647556	8.569362
Pb	0.000730	0.000311	4.285281
Pb	4.415224	6.323744	0.001157
Pb	8.829627	6.323720	4.284552
I	4.208561	3.162013	8.017124
I	4.623167	9.486026	0.553958
I	0.189945	9.486769	3.725459
I	8.627121	3.164862	4.840764
I	1.607680	0.216754	1.517624
I	7.240016	12.446733	7.056293
I	2.819191	12.428739	5.797767
I	6.023001	0.216097	2.766849
I	7.223730	6.541354	7.053261
I	1.591225	6.122609	1.514348
I	6.005376	6.095950	2.779014
I	2.807906	6.540038	5.803033
N	8.401957	9.490763	0.151379
N	0.427966	3.165495	8.417808

N	4.840568	3.151106	4.445914
N	3.985092	9.480288	4.126383
C	8.011253	3.169737	0.668532
C	0.820180	9.494269	7.903087
C	5.234213	9.482884	4.945276
C	3.596318	3.154711	3.620017
H	4.953442	9.483459	6.007432
H	5.807210	10.386344	4.703169
H	5.809920	8.580820	4.704690
H	3.411562	10.322300	4.349601
H	3.414547	8.636320	4.350067
H	4.188149	9.480532	3.101819
H	3.021433	4.057409	3.860551
H	3.019776	2.251732	3.855026
H	3.883449	3.157741	2.559601
H	4.633006	3.149587	5.469582
H	5.414918	3.993813	4.227252
H	5.413228	2.308264	4.223383
H	7.441700	4.076416	0.430940
H	8.294370	3.165242	1.729921
H	7.431934	2.270796	0.425558
H	0.998181	2.321194	0.070442
H	1.002495	4.006882	0.070297
H	0.223659	3.165984	7.393584
H	0.539334	9.492205	6.841094
H	1.397506	8.593932	8.145537
H	1.390911	10.399416	8.143891
H	8.604490	9.489847	1.175997
H	7.831293	8.647303	8.496742
H	7.828881	10.333112	8.498917