Supporting information for:

Atomistic origins of high-performance in hybrid halide perovskite solar cells

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A dataset comprised of GAUSSIAN input and output files used in this work are electronically available as a figshare dataset `http://dx.doi.org/10.6084/m9.figshare.915406`.[S1]

The files comprise of geometry optimisations of methylammonia [MA] (including flourinated analogues [MA-1F, MA-2F, MA-3F]), ammonia [NH4] and formamidinium [forma]. Structures were relaxed at B3LYP/6-31G*, and the polarisation tensor was calculated at B3LYP/6-31G* and CCSD/CC-PVQZ. A PCM prefix to the filename indicates that the calculation (geometry relaxation and single point) was carried out with the polarizable continuum model (PCM) with Ethanol as the solvent.

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References

(S1) Figshare data set. http://dx.doi.org/10.6084/m9.figshare.915406.