

AUTHOR CORRECTION

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Author Correction: Machine-learned impurity level prediction for semiconductors: the example of Cd-based chalcogenides

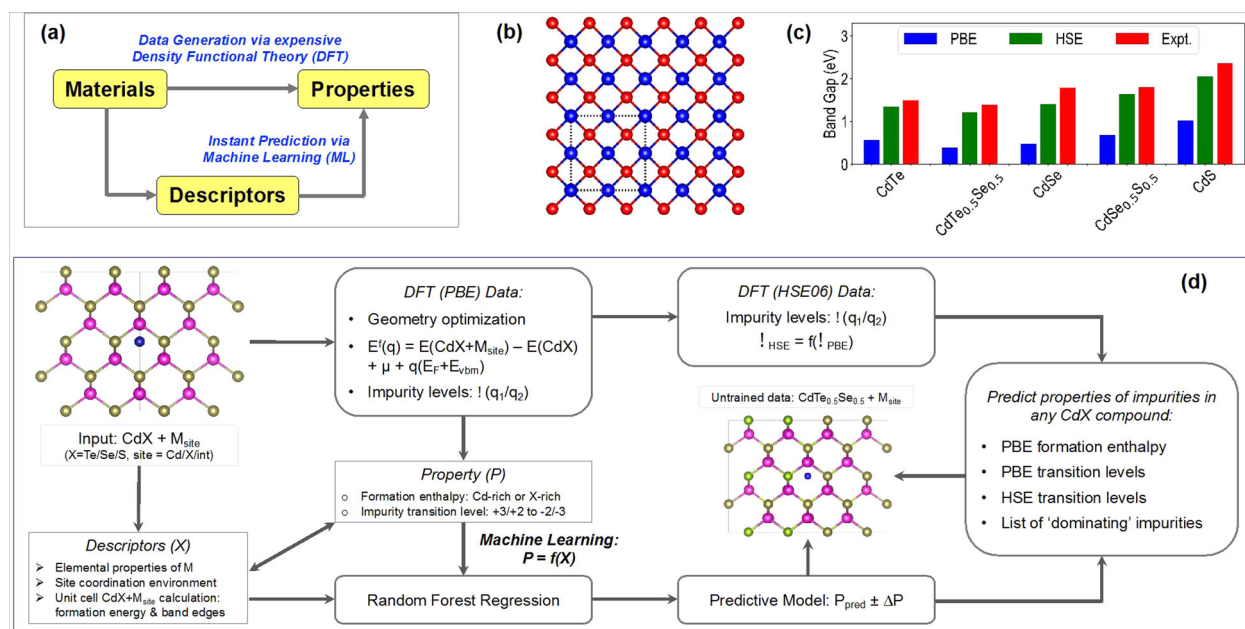
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npj Computational Materials (2020)6:134; <https://doi.org/10.1038/s41524-020-00400-9>

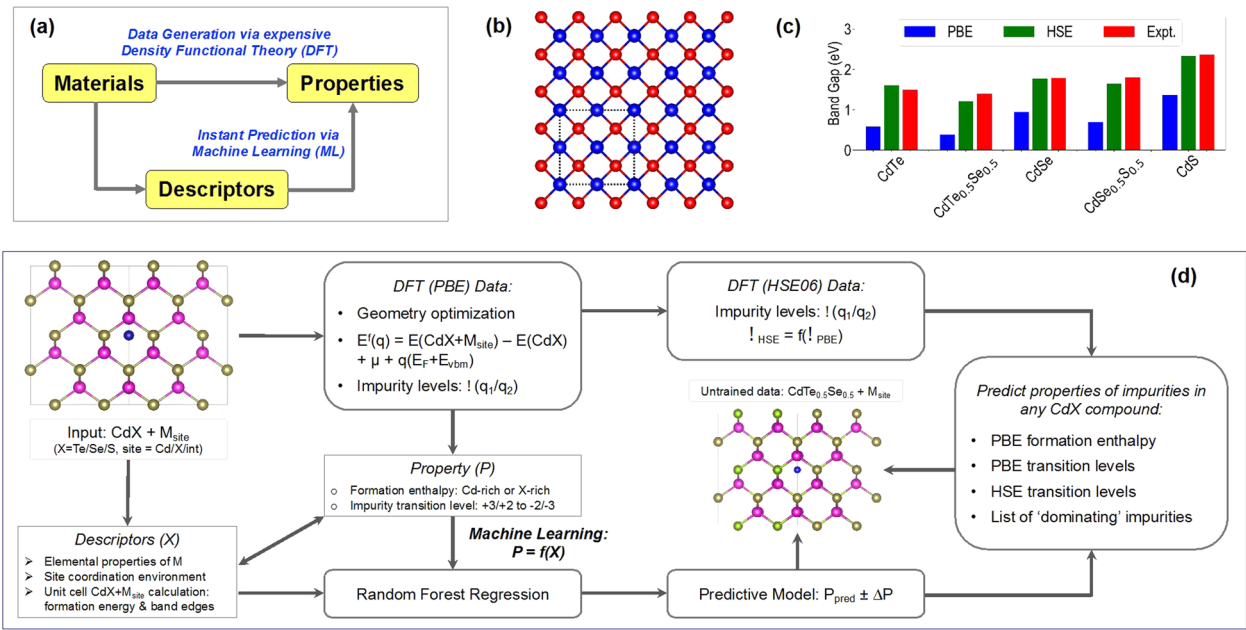
Correction to: npj Computational Materials <https://doi.org/10.1038/s41524-020-0296-7>, published online 23 April 2020

The authors became aware of a mistake in the original version of this Article. Specifically, some of the band gap values plotted and reported in Fig. 1c and Table SI-1 were incorrect. This error originated because two different types of k-point meshes were used in DFT computations performed on CdTe, CdSe and CdS: one which is gamma-centered and one which is not gamma-centered. The gamma-centered calculation results are the correct quantities; the non-gamma-centered results were mistakenly reported in the original versions of Fig. 1 and Table SI-1. As a result of this, the following changes have been made to the originally published version of this Article:

The correct version of Fig. 1:



replaces the previous incorrect version:



The correct version of Table SI-1:

| Compound | Lattice constant (Å) | PBE Band Gap (eV) | HSE Band Gap (eV) |
|---------------------------------------|----------------------|-------------------|-------------------|
| CdTe | 6.63 | 0.57 | 1.34 |
| CdTe _{0.5} Se _{0.5} | 6.42 | 0.39 | 1.21 |
| CdSe | 6.21 | 0.48 | 1.41 |
| CdSe _{0.5} S _{0.5} | 6.07 | 0.70 | 1.64 |
| CdS | 5.94 | 1.03 | 2.05 |

| System | Calculation | Lattice Constant (Å) | Band Gap (eV) |
|------------------|---|----------------------|---------------|
| CdTe | PBE_relaxed | 6.63 | 0.57 |
| CdTe | HSE (on PBE_relaxed) | 6.63 | 1.34 |
| CdTe | HSE_relaxed | 6.56 | 1.44 |
| CdTe | Expt -> Sol. Energy Mater. Sol. Cells, 159, 389-394 (2017) | 6.48 | 1.50 |
| CdTe | Expt -> Science and Technology of Adv. Mater., 19:1, 683-692 (2017) | 6.49 | 1.50 |
| CdTe | Theory -> Semicond. Sci. Technol. 31, 083002 (2016) | 6.58 | 1.49 |
| CdTe | Theory -> Chin. Phys. B, 28, 8, 086106 (2019) | 6.55 | 1.52 |
| CdSe | PBE_relaxed | 6.21 | 0.48 |
| CdSe | HSE (on PBE_relaxed) | 6.21 | 1.41 |
| CdSe | HSE_relaxed | 6.15 | 1.48 |
| CdSe | Expt -> Sol. Energy Mater. Sol. Cells, 159, 389-394 (2017) | 6.08 | 1.70 |
| CdSe | Expt -> Science and Technology of Adv. Mater., 19:1, 683-692 (2017) | 6.00 | 1.74 |
| CdSe | Theory -> Chin. Phys. B, 28, 8, 086106 (2019) | 6.13 | 1.69 |
| CdSeTe (ordered) | PBE_relaxed | 6.41 | 0.39 |
| CdSeTe (ordered) | HSE (on PBE_relaxed) | 6.41 | 1.21 |
| CdSeTe (ordered) | HSE_relaxed | 6.36 | 1.28 |
| CdSeTe (SQS) | PBE_relaxed | 6.42 | 0.39 |
| CdSeTe (SQS) | HSE (on PBE_relaxed) | 6.42 | 1.21 |
| CdSeTe (SQS) | HSE_relaxed | 6.36 | 1.30 |
| CdSeTe | Expt. Literature | 6.25 | 1.42 |

replaces the previous incorrect version:

| Compound | Lattice constant (Å) | PBE Band Gap (eV) | HSE Band Gap (eV) |
|---------------------------------------|----------------------|-------------------|-------------------|
| CdTe | 6.63 | 0.59 | 1.61 |
| CdTe _{0.5} Se _{0.5} | 6.42 | 0.39 | 1.21 |
| CdSe | 6.21 | 0.95 | 1.77 |
| CdSe _{0.5} S _{0.5} | 6.07 | 0.70 | 1.65 |
| CdS | 5.94 | 1.37 | 2.33 |

| System | Calculation | Lattice Constant (Å) | Band Gap (eV) |
|--------|--|----------------------|---------------|
| CdTe | This work PBE_relaxed | 6.63 | 0.59 |
| CdTe | This work HSE (on PBE_relaxed) | 6.63 | 1.61 |
| CdTe | This work HSE_relaxed | 6.56 | 1.44 |
| CdTe | Expt. Literature Expt -> Sol. Energy Mater. Sol. Cells, 159, 389-394 (2017) | 6.48 | 1.50 |
| CdTe | Expt. Literature Expt -> Science and Technology of Adv. Mater., 19:1, 683-692 (2017) | 6.49 | 1.50 |
| CdTe | Theory Literature Theory -> Semicond. Sci. Technol. 31, 083002 (2016) | 6.58 | 1.49 |
| CdTe | Theory Literature Theory -> Chin. Phys. B. 28, 8, 086106 (2019) | 6.55 | 1.52 |

| System | Calculation | Lattice Constant (Å) | Band Gap (eV) |
|--------|--|----------------------|---------------|
| CdSe | This work PBE_relaxed | 6.21 | 0.95 |
| CdSe | This work HSE (on PBE_relaxed) | 6.21 | 1.77 |
| CdSe | This work HSE_relaxed | 6.15 | 1.65 |
| CdSe | Expt. Literature Expt -> Sol. Energy Mater. Sol. Cells, 159, 389-394 (2017) | 6.08 | 1.70 |
| CdSe | Expt. Literature Expt -> Science and Technology of Adv. Mater., 19:1, 683-692 (2017) | 6.00 | 1.74 |
| CdSe | Theory Literature Theory -> Chin. Phys. B. 28, 8, 086106 (2019) | 6.13 | 1.69 |

| System | Calculation | Lattice Constant (Å) | Band Gap (eV) |
|------------------|--|----------------------|---------------|
| CdSeTe (ordered) | This work PBE_relaxed | 6.41 | 0.39 |
| CdSeTe (ordered) | This work HSE (on PBE_relaxed) | 6.41 | 1.21 |
| CdSeTe (ordered) | This work HSE_relaxed | 6.36 | 1.28 |
| CdSeTe (SQS) | This work PBE_relaxed | 6.42 | 0.39 |
| CdSeTe (SQS) | This work HSE (on PBE_relaxed) | 6.42 | 1.21 |
| CdSeTe (SQS) | This work HSE_relaxed | 6.36 | 1.30 |
| CdSeTe | Expt. Literature Expt -> Science and Technology of Adv. Mater., 19:1, 683-692 (2017) | 6.25 | 1.42 |

These errors have been corrected in the PDF and HTML versions of the Article, and the HTML has been updated to include a corrected version of the Supplementary Information.

The band gaps and band edges used in the remainder of the manuscript are correct and no other results are affected. We thank Maciej Piotr Polak of the University of Wisconsin Madison for the reporting of this error.

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