

M. Sitaula et al., Solar Energy Materials and Solar Cells. 306, 114514 (2026), Supplementary Material

## **Computational study of intrinsic defects and photoluminescence spectra in CdTe**

M. Sitaula <sup>a</sup>, V. T. Barone <sup>a</sup>, B. K C <sup>a</sup>, B. R. Tuttle <sup>b</sup>, R. J. Ellingson <sup>a</sup>, S. V. Khare <sup>a\*</sup>

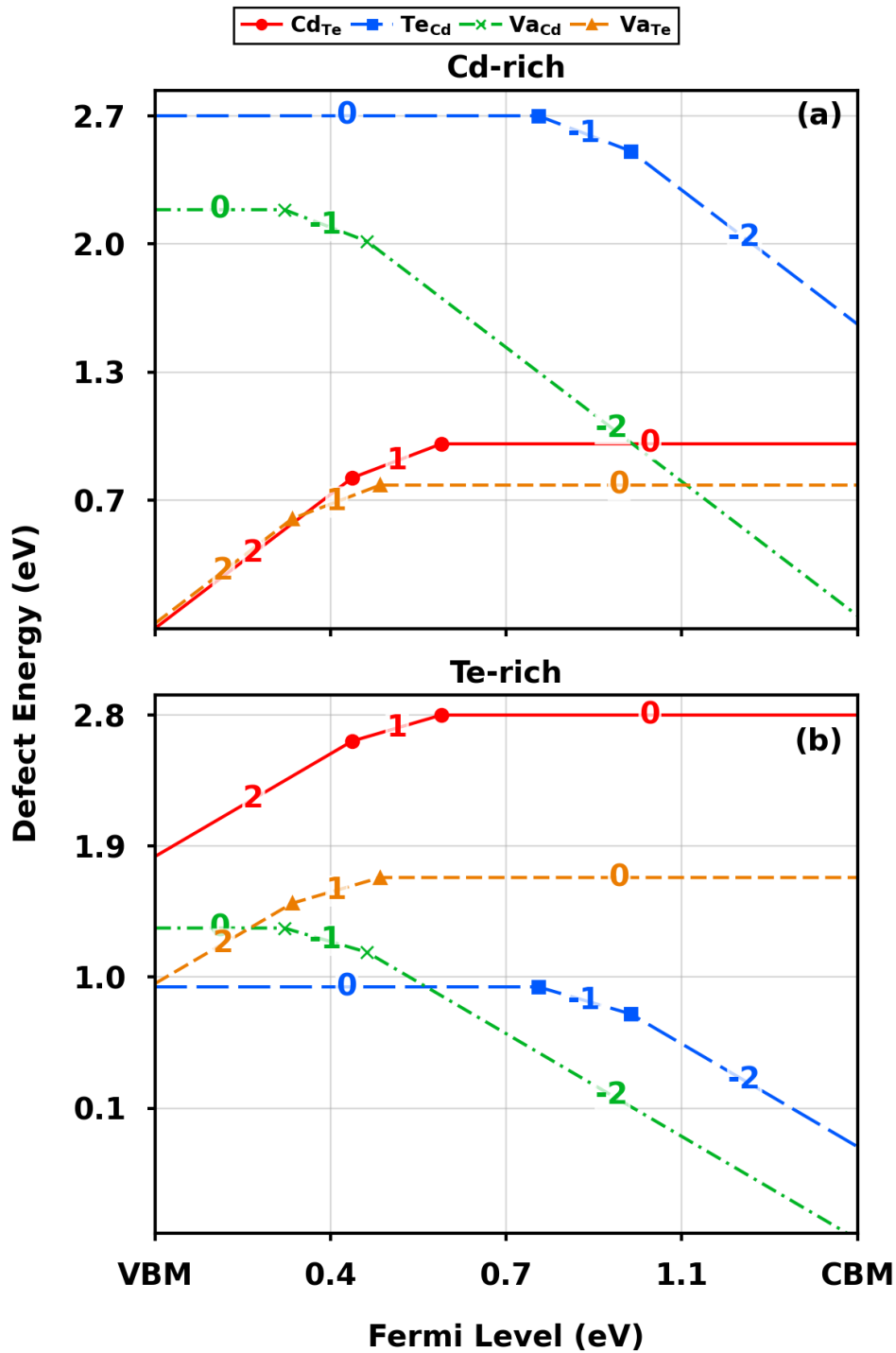
<sup>a</sup>Department of Physics and Astronomy, and Wright Center for Photovoltaics Innovation and Commercialization (PVIC), University of Toledo, Toledo, OH 43606, USA

<sup>b</sup>Department of Physics, Penn State Behrend, Erie, PA, 16563, USA

\*Corresponding Author: Sanjay. Khare@utoledo.edu

## **Supplementary Material**

**Figure S1:** Calculated defect formation energies (eV) for 64 atom CdTe supercells presented in panels (a) and (b) under Cd-rich (a) and Te-rich (b) conditions respectively.



**Table S1:** Relative chemical potentials, Band edges and defect properties for CdTe in 216 atom supercells.

Relative Chemical Potentials:

Scenario	Cd (eV)	Te (eV)
A	0.00	-0.90
B	-0.90	0.00

Band Edges:

Parameter	Value (eV)
VBM	0.00
CBM	1.42
Supercell VBM	0.42
Supercell CBM	1.01

Defect properties:

Name	Atom I/O	Charge	Energy (eV)	Correction (eV)	Is Shallow
Cd_Te1	Te: -1 Cd: 1	0	2.199	0.000	True
		1	1.564	0.090	True
		2	0.985	0.284	False
		3	0.950	0.539	True
Te_Cd1	Te: 1 Cd: -1	4	0.959	0.884	True
		-4	5.347	0.932	True
		-3	5.651	0.456	True
		-2	3.469	0.150	True
Va_Cd1	Cd: -1	-1	2.771	0.023	True
		0	2.126	0.000	False
		-2	2.567	0.370	False
		-1	2.473	0.130	True
Va_Te1	Te: -1	0	2.423	0.000	True
		0	1.925	0.000	True
		1	1.343	0.072	True
		2	0.817	0.242	False

**Table S2:** Relative chemical potentials, Band edges and defect properties for CdTe in 64 atom supercells.

Relative Chemical Potentials:

Scenario	Cd (eV)	Te (eV)
A	0.00	-0.90
B	-0.90	0.00

Band Edges:

Parameter	Value (eV)
VBM	0.00
CBM	1.42
Supercell VBM	0.44
Supercell CBM	1.02

Defect properties:

Name	Atom I/O	Charge	Energy (eV)	Correction (eV)	Is Shallow
Cd_Te1	Te: -1 Cd: 1	0	1.873	0.000	True
		1	1.223	0.071	True
		2	0.613	0.284	False
		3	0.685	0.589	True
		4	0.799	0.997	True
Te_Cd1	Te: 1 Cd: -1	-4	5.305	1.126	
		-3	5.643	0.498	True
		-2	3.433	0.105	True
		-1	2.595	-0.017	True
		0	1.803	0.000	False
Va_Cd1	Cd: -1	-2	2.299	0.600	False
		-1	2.233	0.237	True
		0	2.209	0.000	True
Va_Te1	Te: -1	0	1.655	0.000	True
		1	1.185	0.015	True
		2	0.760	0.162	False