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Effects of short-range order in phase equilibria and opto-electronic properties of ternary alloy $Zn_xCd_{1-x}Te$

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Table S1: Equilibrium lattice parameters and formation energies of $Zn_xCd_{1-x}Te$ alloys per formula unit in B3 crystal structure, computed using GGA functional. Values from the literature are listed where available.

Material	Lattice Constant a (Å)	Volume V (Å^3)	Formation Energy (eV)
CdTe	6.62, 6.48[a], 6.54[b]	290.12	- 0.96
$Zn_{0.25}Cd_{0.75}Te$	6.52	277.17	- 0.95
$Zn_{0.50}Cd_{0.50}Te$	6.42, 6.365[c]	264.61	- 0.95
$Zn_{0.75}Cd_{0.25}Te$	6.30	250.05	- 0.95
ZnTe	6.18, 6.08[d], 6.1026[e]	236.03	- 0.97

[a]Theoretical Ref. [1]
[b]Experimental Ref. [2]
[c]Experimental Ref. [3]
[d]Theoretical Ref. [4]
[e]Experimental Ref. [5]

Table S2: Electronic band gaps of $Zn_xCd_{1-x}Te$ alloys, calculated implementing GGA and hybrid HSEO6 functionals. Values from the literature are listed where available.

Material	Band Gap, Direct (eV)		
	GGA	HSEO6	Other Works
CdTe	0.94	1.54	1.31[a], 1.50[b]
$Zn_{0.25}Cd_{0.75}Te$	0.99	1.49	-
$Zn_{0.50}Cd_{0.50}Te$	1.05	1.60	-
$Zn_{0.75}Cd_{0.25}Te$	1.15	1.77	-
ZnTe	1.28	2.39	2.24[c,d], 2.39[e,f]

[a]Theoretical (FPLAW, EV-GGA) Ref. [6]
[b]Experimental Ref. [7]
[c]Theoretical (LDA) Ref. [1]
[d]Experimental Ref. [8]
[e]Experimental Ref. [9]
[f]Experimental Ref. [10]

Table S3: Average and standard deviation of band structure effective masses (m^*) of electrons and holes of $Zn_xCd_{1-x}Te$ alloys. Values are given in units of electron mass (m_o).

Material	Electron Effective Mass (m_e^*)		Hole Effective Mass (m_h^*)	
	Average	Standard Deviation	Average	Standard Deviation
CdTe	1.33	1.01	0.17	0.10
$Zn_{0.25}Cd_{0.75}Te$	1.56	0.88	0.35	0.26
$Zn_{0.50}Cd_{0.50}Te$	1.74	1.05	0.37	0.28
$Zn_{0.75}Cd_{0.25}Te$	1.53	0.94	0.40	0.32
ZnTe	1.20	0.94	0.17	0.10

Table S4: Charge transfer from Cd and Zn to Te in $Zn_xCd_{1-x}Te$ alloys computed using the Bader charge segregation scheme [11-14]. Values are given in elementary charge units.

Material	Cd	Zn
CdTe	0.52	N/A
$Zn_{0.25}Cd_{0.75}Te$	0.51	0.52
$Zn_{0.50}Cd_{0.50}Te$	0.51	0.52
$Zn_{0.75}Cd_{0.25}Te$	0.50	0.51
ZnTe	N/A	0.50

Table S5: Dielectric constants of $Zn_xCd_{1-x}Te$ alloys calculated using the hybrid HSEO6 functional.

Material	Dielectric Constant
CdTe	5.87
$Zn_{0.25}Cd_{0.75}Te$	6.36
$Zn_{0.50}Cd_{0.50}Te$	6.45
$Zn_{0.75}Cd_{0.25}Te$	6.53
ZnTe	6.04

Table S6: Charge carrier mobility, Urbach Energy, and Exciton Binding Energy of $Zn_xCd_{1-x}Te$ alloys calculated using the hybrid HSEO6 functional.

Material	Hole Mobility (cm^2/Vs)	Electron Mobility (cm^2/Vs)	Urbach Energy (meV)	Exciton Binding Energy (meV)
CdTe	103.42, 100[a]	13.21	18.94, 15[c]	45.01
$Zn_{0.25}Cd_{0.75}Te$	50.23	11.27	21.97	96.46
$Zn_{0.50}Cd_{0.50}Te$	47.52	10.10	20.72	97.86
$Zn_{0.75}Cd_{0.25}Te$	43.95	11.49	21.17	83.09
ZnTe	103.42, 100[b]	14.65	23.08	91.62

[a]Experimental Ref. [15] (At 225 K temperature)
[b]Experimental Ref. [16] (At 275 K temperature)
[c]Experimental Ref. [17]

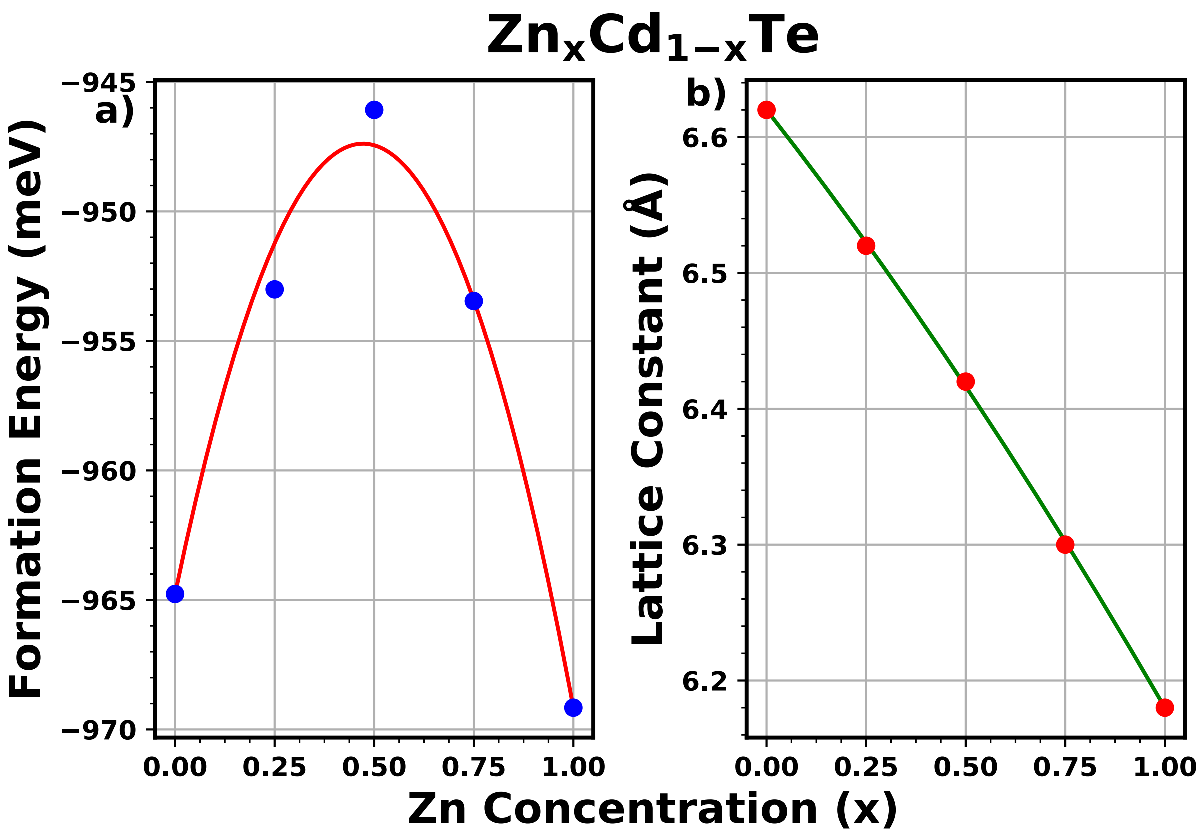

Figure S1: a) Formation energies, and b) lattice constants of $Zn_xCd_{1-x}Te$ alloys calculated using the GGA functional. Here, points denote calculated values whereas curves sketch fitting based on a bowing parameter defined in Eq. (3).

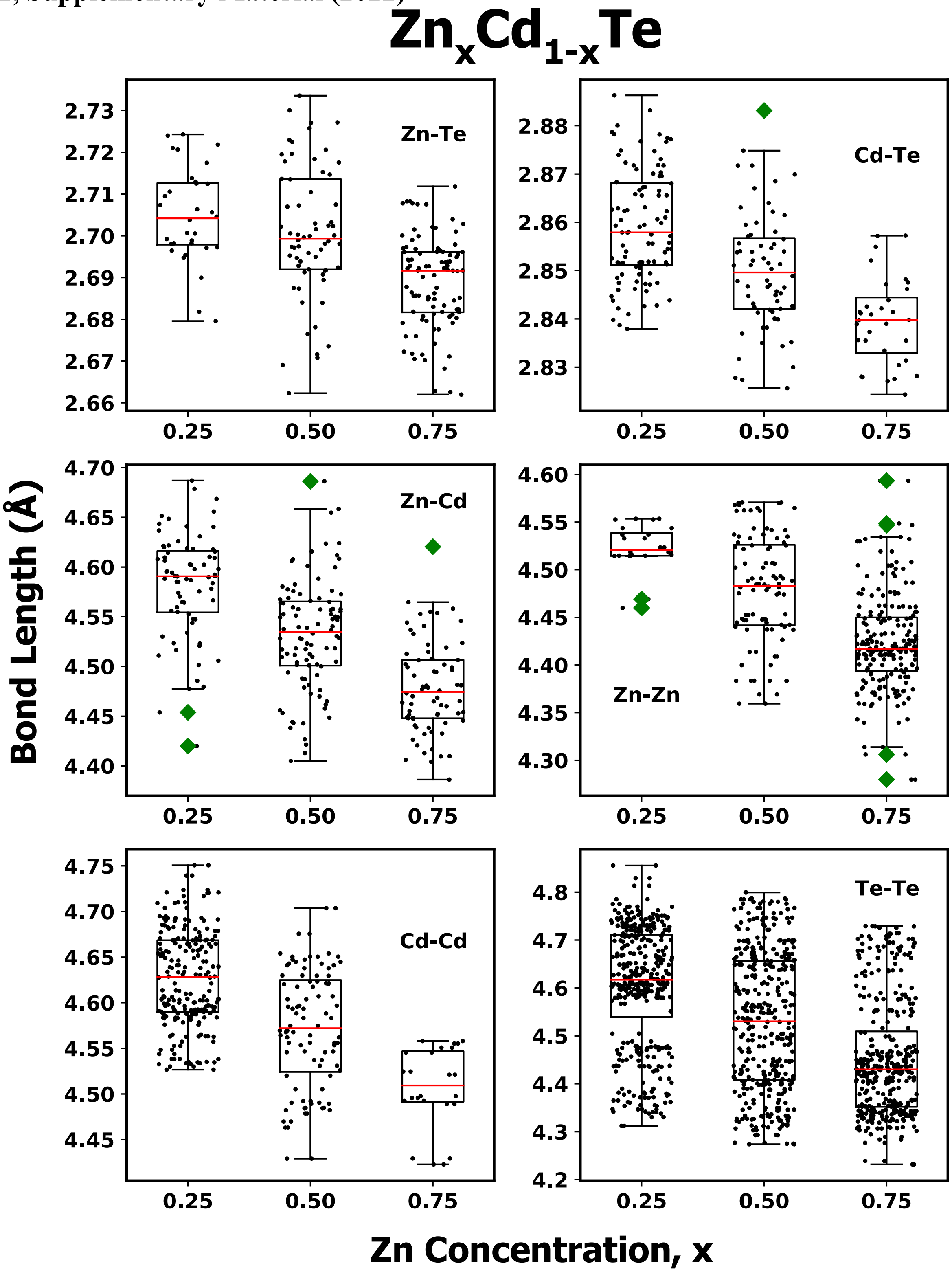

Figure S2: Box-and-whisker plots displaying the distribution of various first nearest neighbor bond lengths (Zn-Te, Cd-Te, Zn-Cd, Zn-Zn, Cd-Cd and Te-Te) at intermediate Zn concentrations (x = 0.25, 0.50, 0.75) within disordered $Zn_xCd_{1-x}Te$ alloys, simulated using SQS. Horizontal red lines denote the median whereas the green diamonds denote the outliers.

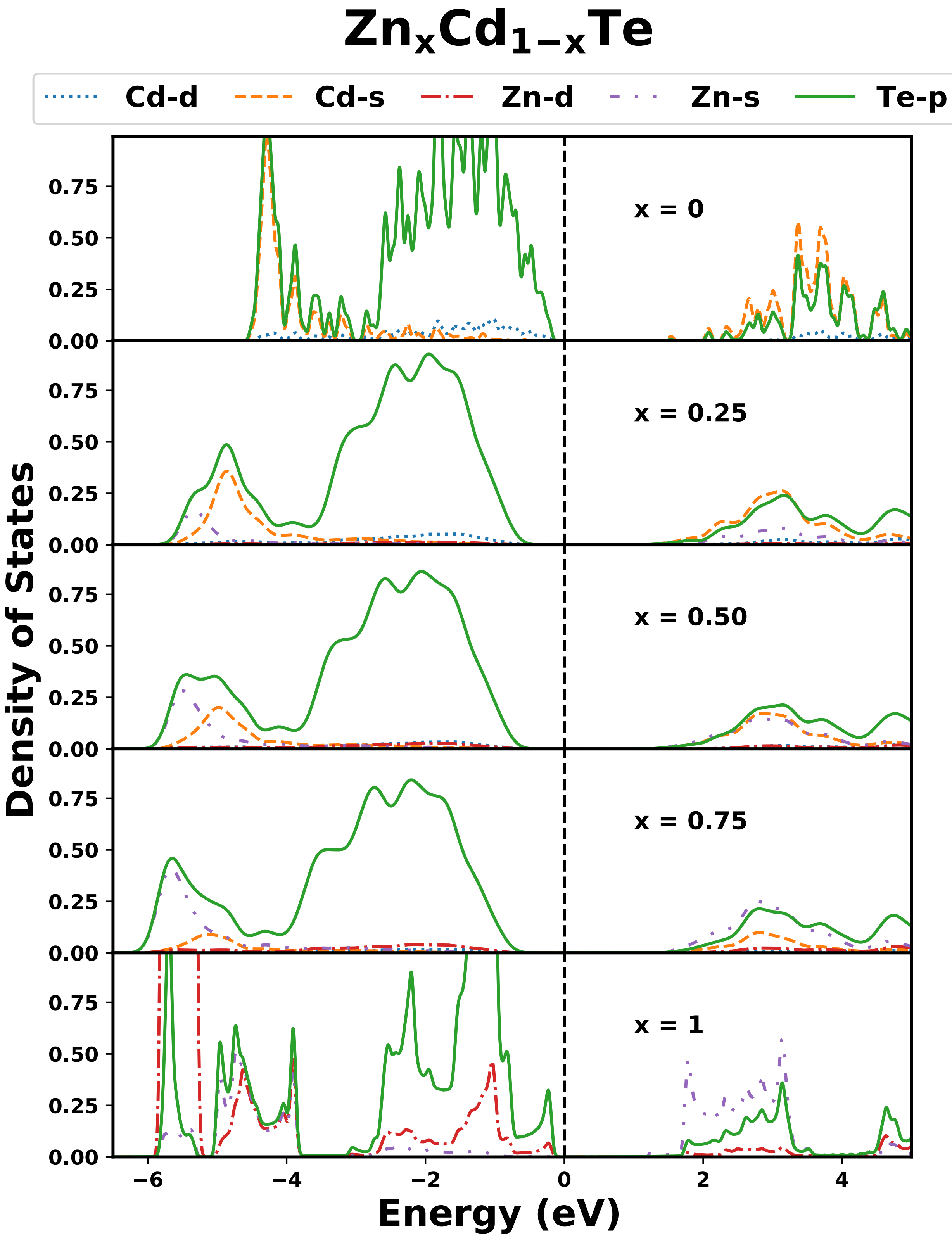

Fig S3: On-site projected electronic density of states (PDOS) per formula unit of $Zn_xCd_{1-x}Te$ alloys calculated using the HSE06 functional. The Fermi level is set to 0 eV.

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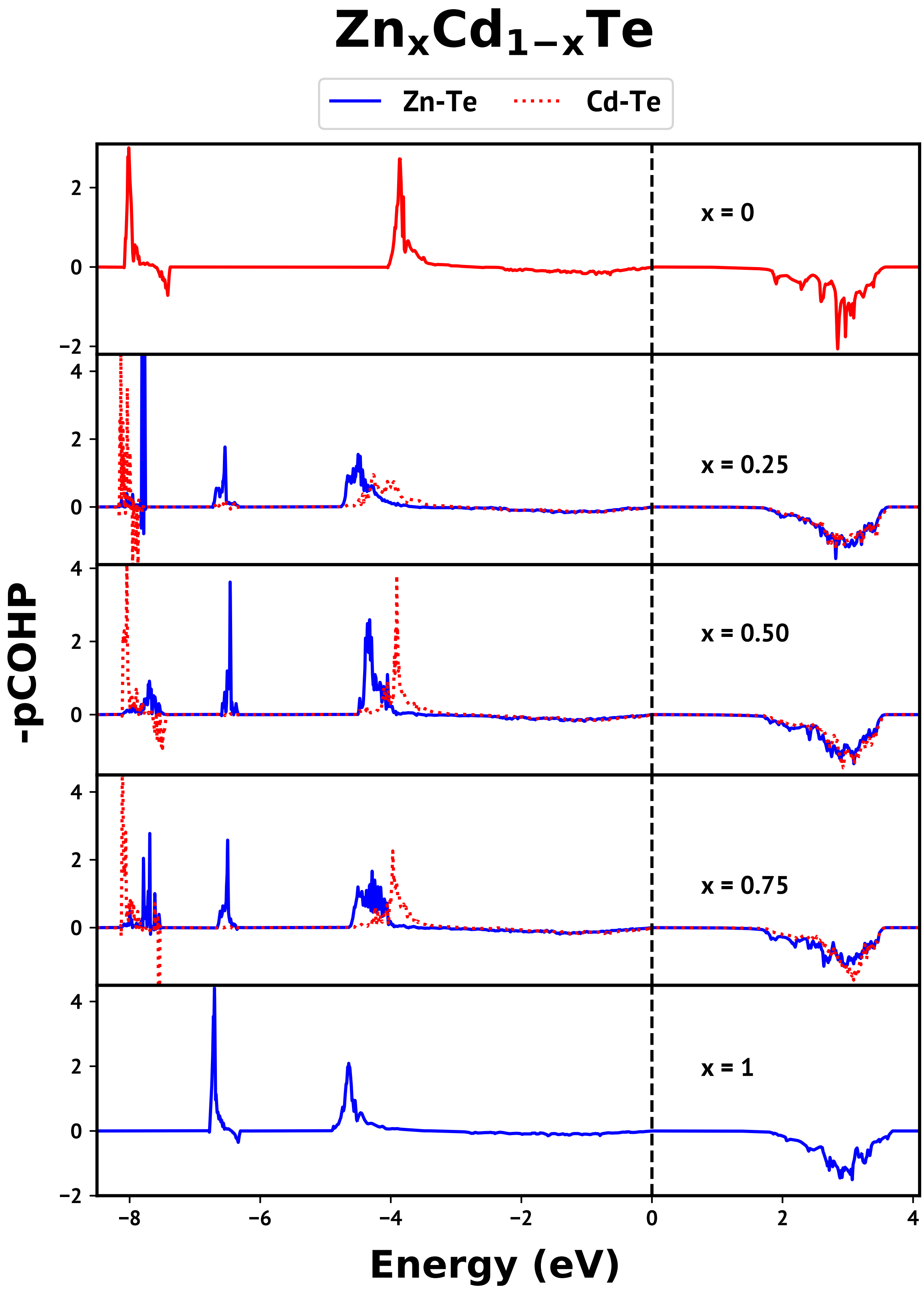

Figure S4: Projected Crystal Orbital Hamiltonian Populations (-pCOHP) of nearest-neighbors' interactions of $Zn_xCd_{1-x}Te$ alloys. All other covalent interactions are negligible compared to Cd-Te and

Zn-Te pairs displayed here. Positive and negative values of -pCOHP correspond to bonding and antibonding interactions respectively. The Fermi level is set to 0 eV.

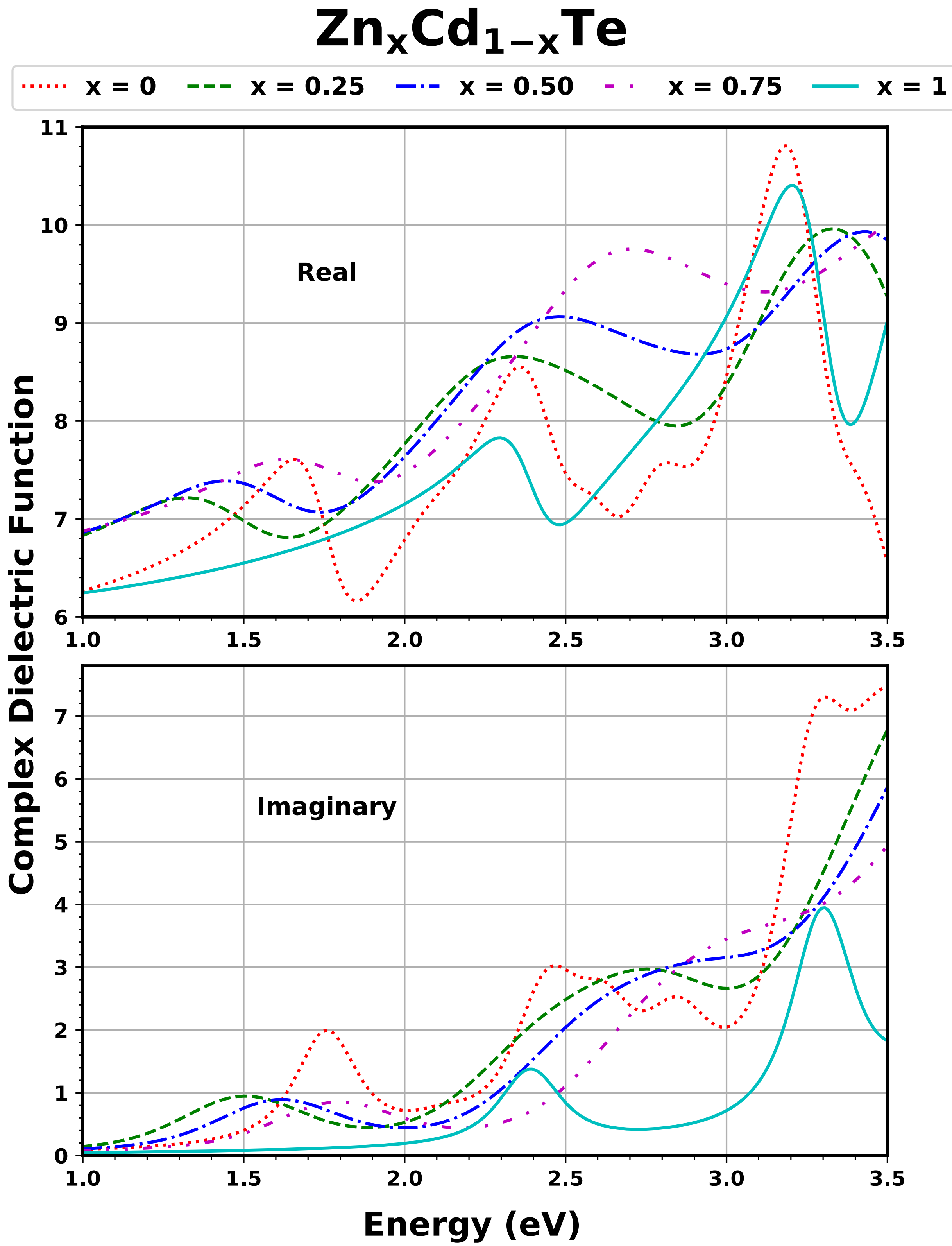

Figure S5: Complex dielectric functions of $Zn_xCd_{1-x}Te$ alloys computed utilizing the hybrid HSEO6 functional. Photon energies shown are in the visible-UV range.

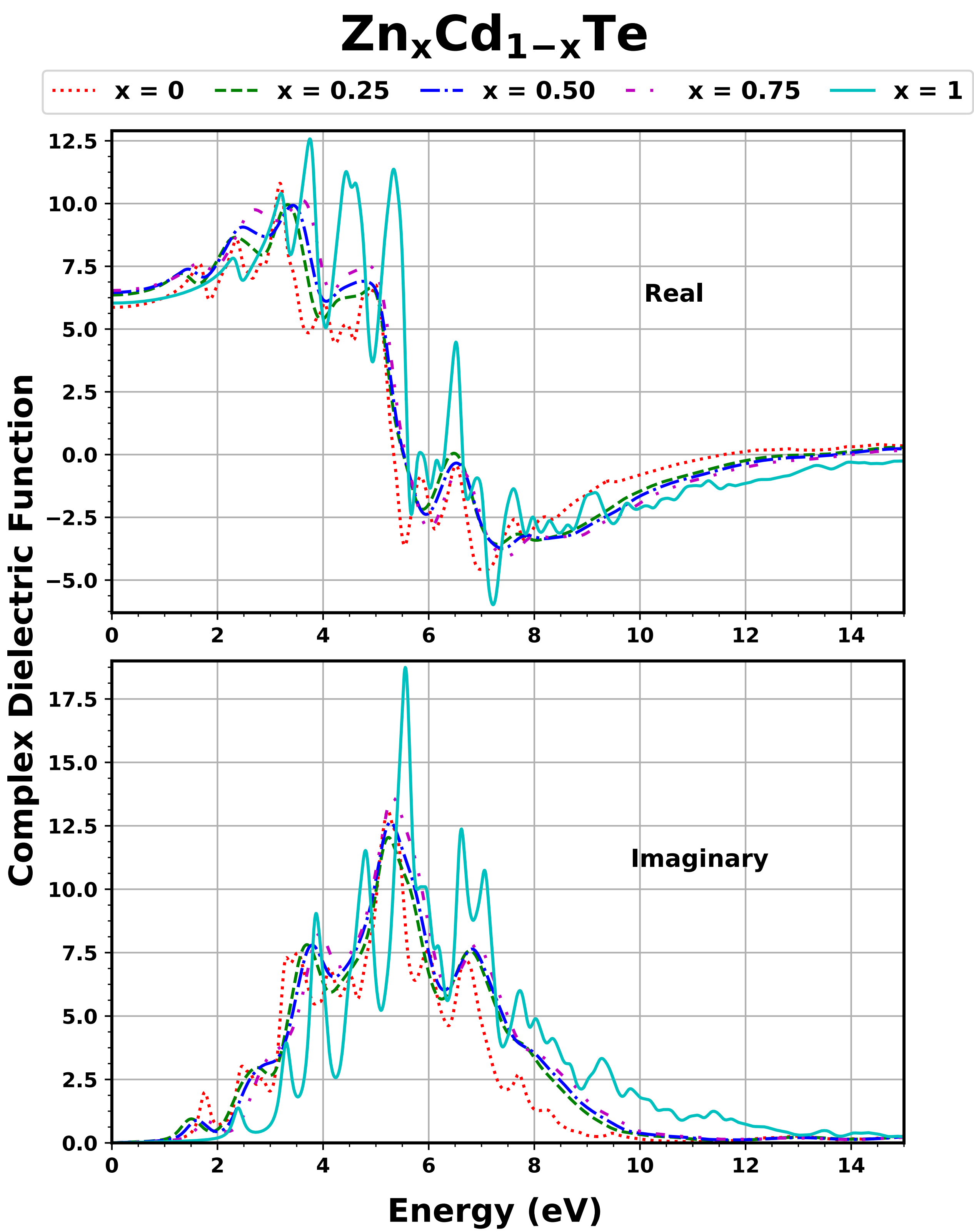
$Zn_xCd_{1-x}Te$
x = 0
x = 0.25
x = 0.50
x = 0.75
x = 1
Real
Imaginary
Complex Dielectric Function
Energy (eV)

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Figure S6: Variation of complex dielectric functions of $Zn_xCd_{1-x}Te$ alloys, calculated using the hybrid HSEO6 functional. Photon energies shown are in the range (0-15) eV.

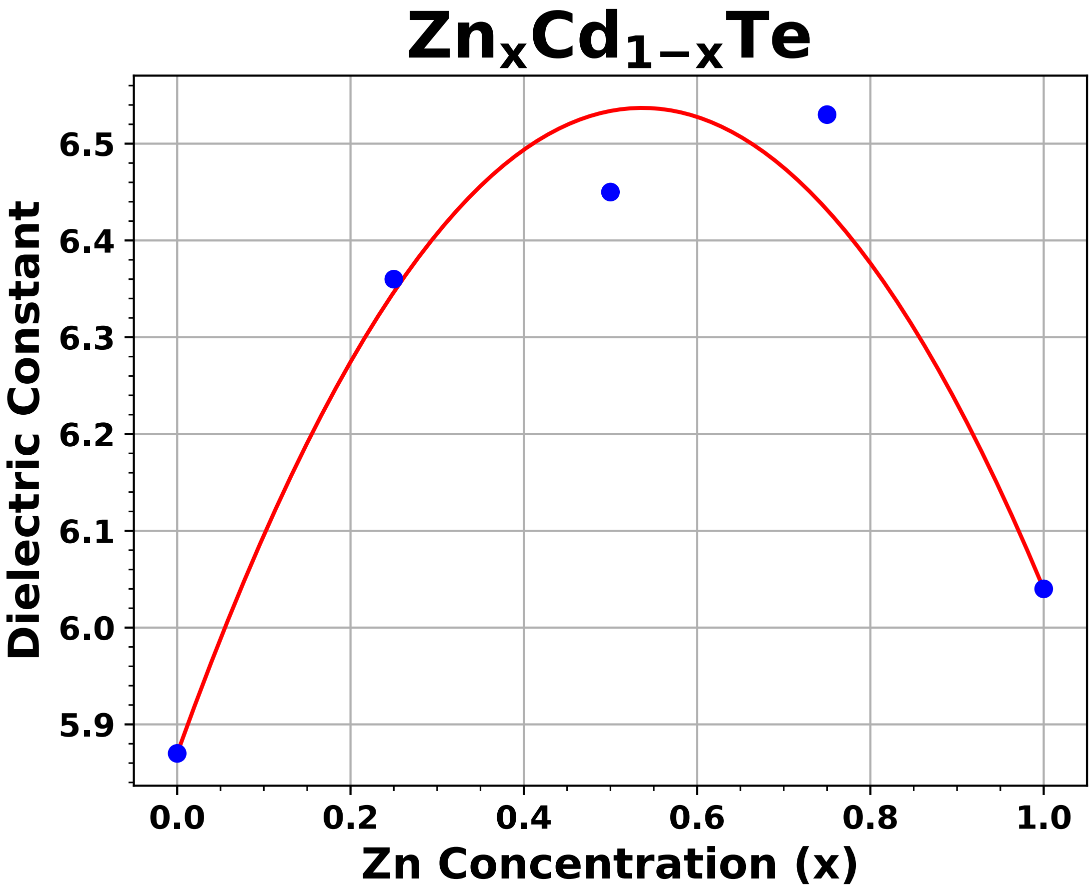

Figure S7: Dielectric constants of $Zn_xCd_{1-x}Te$ alloys calculated using the hybrid HSEO6 functional. Here, points denote calculated values whereas curves sketch fitting based on a bowing parameter defined in Eq. (3).

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