The thermoelectric properties of CdBr, CdI, and Janus Cd_2BrI monolayers with low lattice thermal conductivity

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Abstract: The investigation and development of high thermoelectric value materials has become a research hotspot in recent years. In this work, based on the density functional theory in the Perdew-Burke-Ernzerhof (GGA-PBE) level, the thermoelectric properties of transition metal halides CdBr, Janus Cd_2BrI, and CdI monolayers have been systematically investigated using Boltzmann transport theory. The calculation of electronic band structure shows that these three materials have indirect band gap semiconductor properties. For carrier transport, the electron mobility for CdBr, Janus Cd_2BrI, and CdI monolayers are found to be 74, 16, 21 $cm^2s^{-1}V^{-1}$ for *p*-type doping and 116, 102, 78 $cm^2s^{-1}V^{-1}$ for *n*-type doping. Regarding their phonon transport, the CdBr, Cd_2BrI, and CdI monolayers all have very low lattice thermal conductivity (4.78, 2.46, and 1.65 $Wm^{-1}K^{-1}$, respectively) that decreases with increasing temperature, which is

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favorable for obtaining large *zT* values. The electrical transport results show that the performance of *p*-type doping is better than *n*-type doping. At 300 K, the Seebeck coefficients of *p*-type doping for the CdBr, Cd_2BrI, and CdI monolayers are 217.72, 246.43, and 226.24 μV/K, respectively. In addition, we predict the *zT* values of the CdBr, Cd_2BrI, and CdI monolayers are 0.62, 1.64, and 0.87 for *p*-type doping at 300 K respectively. The *zT* values increase with the increase of temperature. In particular, the Janus Cd_2BrI monolayer has a *zT* value of 3.03 at 600 K. These results suggest that all these materials can be good candidates for thermoelectric materials.

Keywords: Thermoelectric, Frist-principles calculations, Electronics structure, MX-type transition metal halides

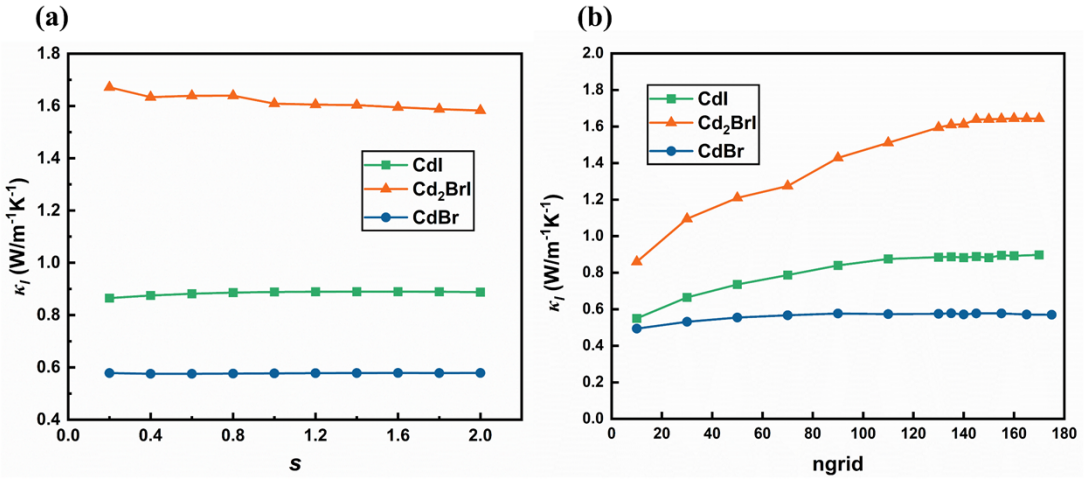

Fig. S1 (Color online) (a)The Gaussian broadening (*s*) and (b)*k* grid convergence curve of the CdBr, Cd_2BrI, and CdI monolayers.

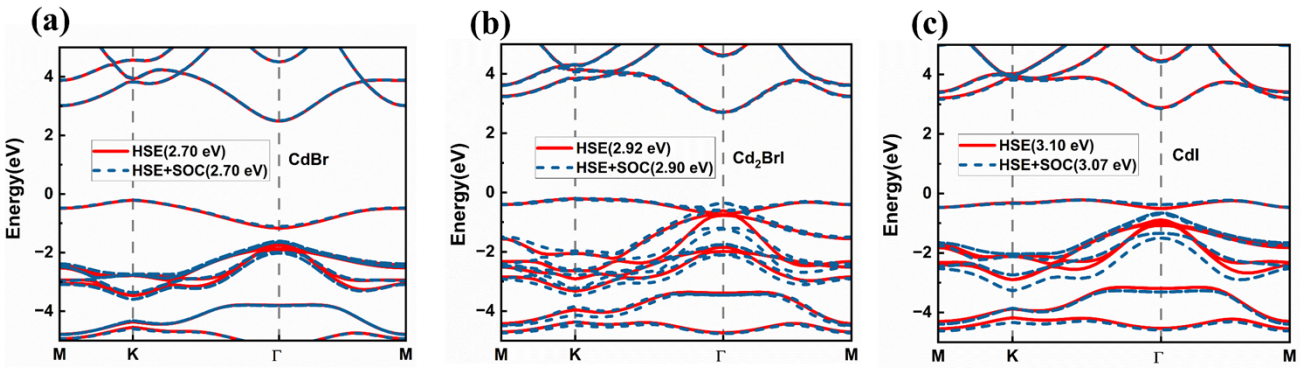

Fig. S2 (Color online) Electronic band structures of the monolayers at the HSE (red lines) and HSE06+SOC (blue dash lines) levels of the CdBr, Cd_2BrI, and CdI monolayers. The VBMs are set to zero.

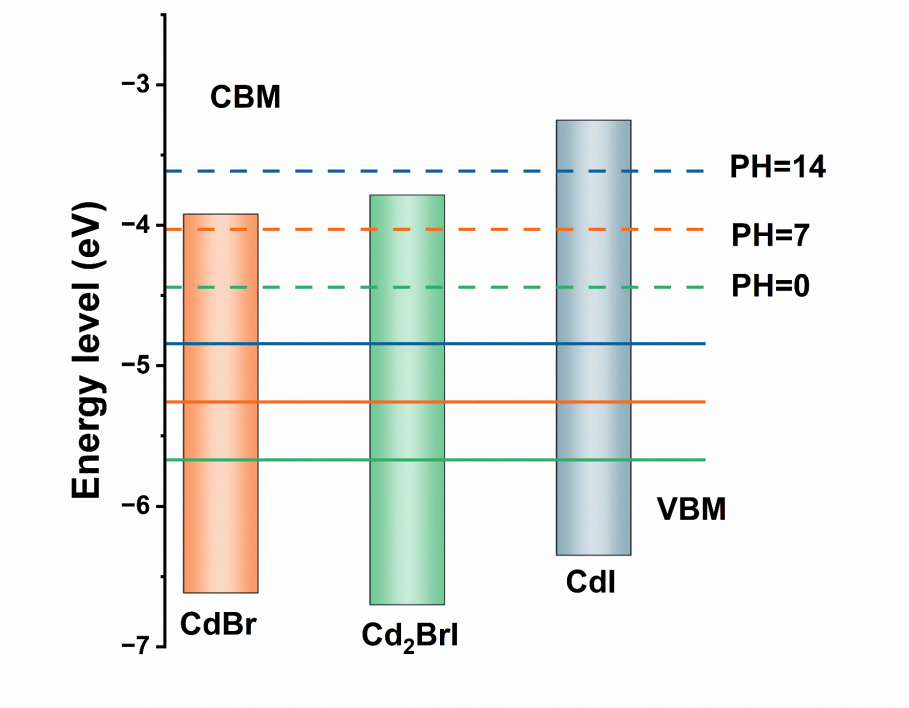

Fig. S3 (Color online) The calculated band edge alignments of the CdBr, Cd_2BrI, and CdI monolayers relative to the vacuum level from the HSE06 functional compared to the redox potential of water splitting at pH = 0, PH = 7, and PH = 14, respectively.

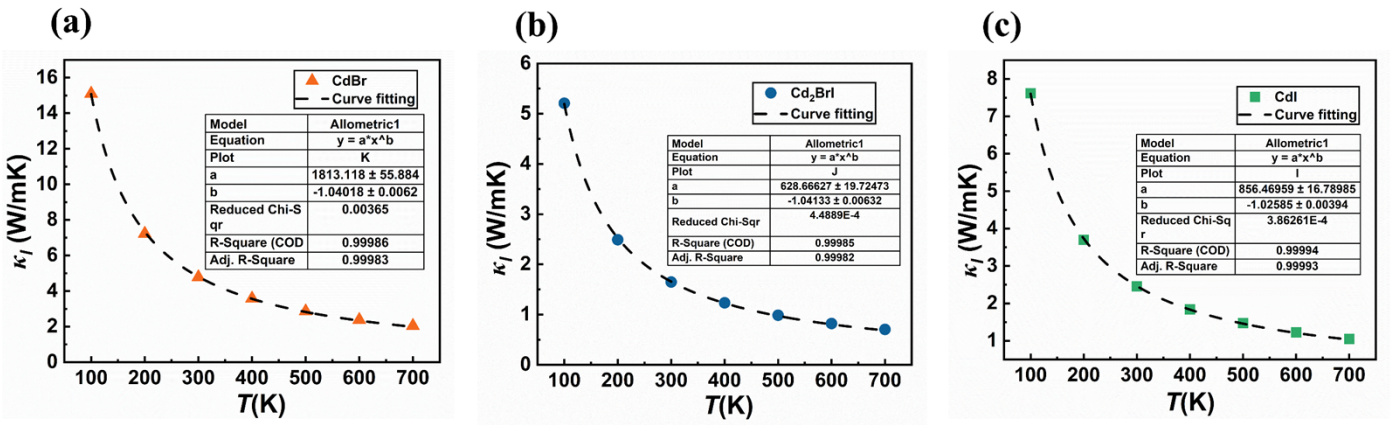

Fig. S4 (Color online) Effective mass under different *k*-points for the CdBr, Cd_2BrI, and CdI monolayers.

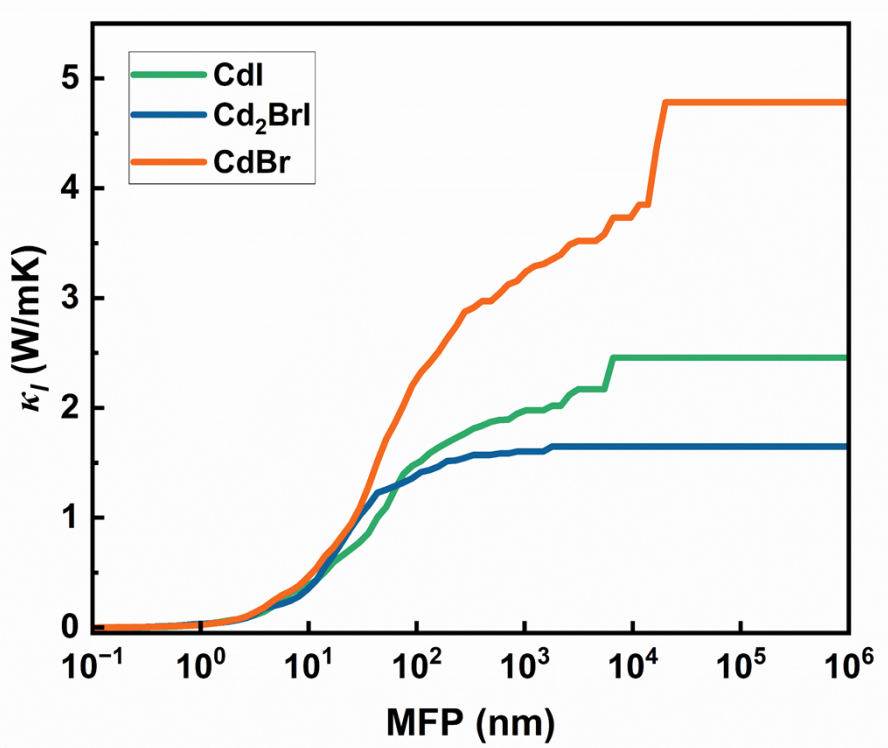

Fig. S5 (Color online) The cumulative κ_l as a function of MFP of the CdBr, Cd_2BrI, and CdI monolayers at 300 K.

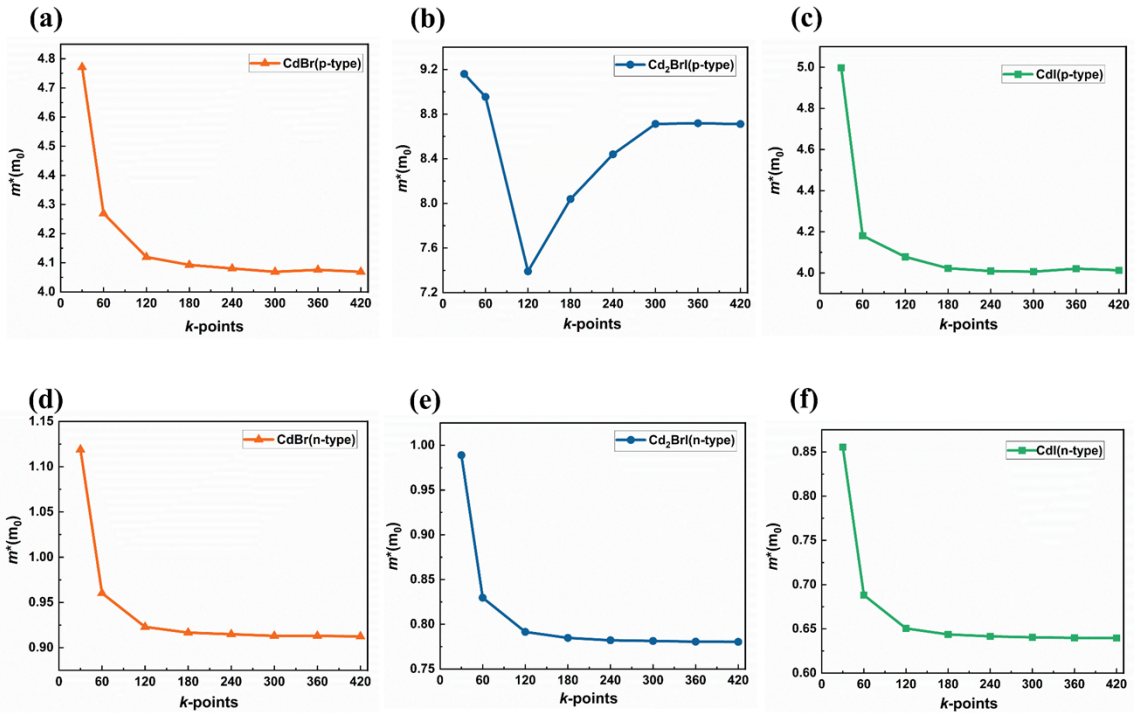

Fig. S6 (Color online) Effective mass under different k-points for the CdBr, Cd_2BrI, and CdI monolayers.

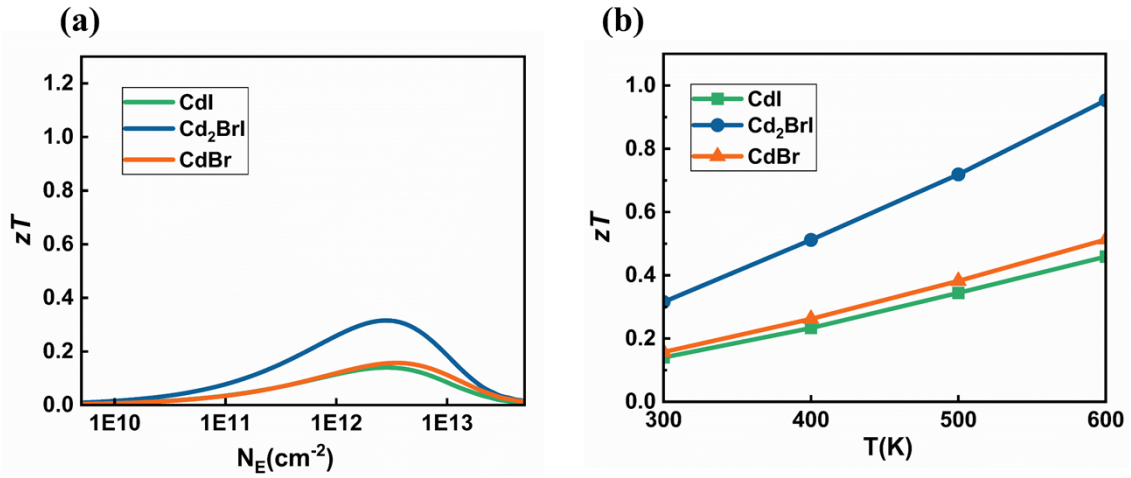

Fig. S7 (Color online) Calculated thermoelectric *zT* as a function of carrier concentration (a) and temperature (b) of the *n*-type doping CdBr, Cd_2BrI, and CdI monolayers.

Table S1 Calculated Seebeck coefficient (*S*), power factors (*PF*), and *zT* values of the CdBr, Cd_2BrI, and CdI monolayers at 300 K and 600 K.

		S (μV/ K)		*PF* (mW/mK^2)		*zT*	
	Types	300 K	600 K	300 K	600 K	300 K	600 K
CdBr	*p*	217.722	250.266	12.179	8.390	0.623	1.538
	n	181.990	210.421	2.714	2.478	0.157	0.513
Cd_2BrI	*p*	246.429	256.345	12.089	5.605	1.640	3.029
	n	202.163	237.726	1.974	1.739	0.316	0.953
CdI	*p*	226.236	237.270	8.744	4.263	0.875	1.706
	n	182.688	210.858	1.230	1.120	0.140	0.459