## Machine-Intelligence-Driven High-Throughput Prediction of 2D Charge Density Wave Phases

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## Supporting Information

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**Table S1:** All CDW materials and their phases, energy differences with the normal phase, and band/CDW-gaps, as found by our computational methodology. Note the convention here. The normal phase is called  $\phi_0$ , the CDW phase just less stable than  $\phi_0$  is called  $\phi_{-1}$ , and the phase just less stable than  $\phi_{-1}$  is named  $\phi_{-2}$ , and so on. Two numbers are in parenthesis beside the  $\phi$  names. The first value denotes the energy difference of that CDW phase with its corresponding normal phase in units of meV/formula unit. The second value states the band/CDW-gap of that CDW phase in units of eV. The CDW-gaps are marked with an asterisk (blue font) while the proper band gaps (red font) are not. For example, the notation  $\phi_{-2}$  (-26.52, 0.5\*) for  $\sqrt{13} \times \sqrt{13}$  periodicities of TaS<sub>2</sub>-T means that this is the 2<sup>nd</sup> CDW phase found in this periodicity by descending order (lower energy is more stable), the phase is more stable than the normal phase by 26.52 meV/formula-unit and it has a 0.5 eV CDW-gap.

Material	2×2	3×3	√13×√13	4×4
TaS <sub>2</sub> -T	No phase	$\phi_{-1}$ (-12, 0)	$\phi_{-1}$ (-13.96, 0)	$\phi_{-1}$ (-17.61, 0)
			$\phi_{-2}$ (-26.52, 0.5*)	
TaS <sub>2</sub> -H	No phase	<i>ф</i> <sub>-1</sub> (-3.92, 0)	$\phi_{-1}$ (-0.22, 0)	$\phi_{-1}$ (-0.42, 0)
			$\phi_{-2}$ (-0.7, 0)	<i>ф</i> <sub>-2</sub> (-1.16, 0)
Hf <sub>3</sub> Te <sub>2</sub>	$\phi_{-1}$ (-2.26, 0)	<i>\$</i> -2 (-2.43, 0)	NA	$\phi_{-1}$ (-0.66, 0)
				$\phi_{-2}$ (-2.72, 0)
LaGeI	$\phi_{-1}$ (-1.62, 0)	No phase	No phase	$\phi_{-1}$ (-2.66, 0)
LaI <sub>2</sub>	No phase	$\phi_{-1}$ (-0.64, 0)	NA	No phase
NbS <sub>2</sub> -T	No phase	<i>\overline{\phi_{-1}}</i> (-9.6, 0)	$\phi_{-1}$ (-38.56, 0.48*)	<i>\overline{\phi_{-1}(-14.11, 0)</i>
NbS <sub>2</sub> -H	<i>ф</i> <sub>-1</sub> (-0.43, 0)	<i>ф</i> <sub>-1</sub> (-0.71, 0)	No phase	$\phi_{-1}$ (-3.9, 0)
	$\phi_{-2}$ (-1.05, 0)	$\phi_{-1}$ (-0.79, 0)		
	$\phi_{-3}$ (-2.77, 0)			
NbSe <sub>2</sub> -T	No phase	<i>ф</i> <sub>-1</sub> (-36.21, 0)	$\phi_{-1}$ (-68.85, 0)	<i>\overline{\phi_{-1}(-33.54, 0)</i>
NbSe <sub>2</sub> -H	$\phi_{-1}$ (-0.22, 0)	<i>φ</i> <sub>-1</sub> (-2.18 0)	$\phi_{-1}$ (-3.31, 0)	$\phi_{-1}$ (-1.78, 0)
	\$\phi_2\$ (-1.05, 0)	$\phi_{-2}(-2.69,0)$		$\phi_{-2}$ (-3.59, 0)
		\$\phi_2 (-2.9, 0)\$		<i>\phi</i> -3 (-4.18, 0)
NbTe <sub>2</sub> -T	No phase	<i>φ</i> <sub>-1</sub> (-87.24, 0)	$\phi_{-1}$ (-93.44, 0)	<i>\phi</i> <sub>-1</sub> (-93.2, 0)

		\$\phi_2\$ (-111.52, 0)		
NbTe <sub>2</sub> -H	$\phi_{-1}$ (-2.02, 0)	$\phi_{-1}$ (-16.81, 0)	$\phi_{-1}$ (-1.08, 0.16*)	$\phi_{-1}$ (-25.08, 0)
			<i>φ</i> <sub>-2</sub> (-4.85, 0.25*)	
OsOCl <sub>2</sub>	$\phi_{-1}$ (-0.58, 0)	No phase	NA	No phase
RuOCl <sub>2</sub>	<i>φ</i> <sub>-1</sub> (-0.13, 0)	No phase	NA	No phase
TaSe <sub>2</sub> -T	No phase	<i>φ</i> <sub>-1</sub> (-43.18, 0)	$\phi_{-1}$ (-67.38, 0.57*)	<i>ф</i> <sub>-1</sub> (-34.95, 0)
TaSe <sub>2</sub> -H	<i>ф</i> <sub>-1</sub> (-0.83, 0)	<i>φ</i> <sub>-1</sub> (-7.16, 0)	$\phi_{-1}$ (-5.72, 0)	$\phi_{-1}$ (-3.2, 0)
	$\phi_{-2}$ (-1.93, 0)	<i>φ</i> <sub>-2</sub> (-8.35, 0)		
		<i>ф</i> -3 (-8.75, 0)		
TaTe <sub>2</sub> -T	No phase	$\phi_{-1}$ (-128.98, 0)	$\phi_{-1}$ (-5.44, 0)	$\phi_{-1}$ (-120.72, 0)
TaTe <sub>2</sub> -H	$\phi_{-1}$ (-6.37, 0)	$\phi_{-1}$ (-18.8, 0)	No phase	<i>\overline{\phi_{-1}}</i> (-22.82, 0)
	<i>φ</i> <sub>-2</sub> (-11.97, 0)	<i>φ</i> <sub>-2</sub> (-23.46, 0)		
Ti <sub>2</sub> PTe <sub>2</sub>	$\phi_{-1}$ (-1.14, 0)	No phase	No phase	No phase
	$\phi_{-1}$ (-1.31, 0)			
TiBr <sub>2</sub>	<i>φ</i> <sub>-1</sub> (-351.36, 0.34)	$\phi_{-1}$ (-178.64, 0)	$\phi_{-1}$ (-286.9, 0.18)	<i>φ</i> <sub>-1</sub> (-353.97, 0.34)
		<i>φ</i> <sub>-2</sub> (-284.93, 0.41)		repeat of 2×2
TiCl <sub>2</sub>	$\phi_{-1}$ (-321.45, 0.38)	<i>ф</i> -1 (-120.01, 0)	$\phi_{-1}$ (-232.63, 0.15)	<i>φ</i> <sub>-1</sub> (-324.81 0.38)
		<i>φ</i> -2 (-216.19, 0.44)		repeat of 2×2
TiOBr	$\phi_{-1}$ (-5.59, 0)	$\phi_{-1}$ (-12.84, 0)	NA	<i>ф</i> <sub>-1</sub> (-11.78, 0)
	$\phi_{-2}$ (-10.86, 0)			
TiOCl	<i>ф</i> <sub>-1</sub> (-7.31, 0)	<i>ф</i> <sub>-1</sub> (-13.6, 0)	NA	<i>\overline{\phi_1\circ}</i> (-20.33, 0.09)
	<i>ф</i> <sub>-2</sub> (-13.37, 0)			
TiS <sub>2</sub>	$\phi_{-1}$ (-5.76, 0.25)	<i>φ</i> <sub>-1</sub> (-2.54, 0.15)	No phase	$\phi_{-1}$ (-4.64, 0.25)
				repeat of 2×2
TiSe <sub>2</sub>	$\phi_{-1}$ (-4.55, 0)	<i>ф</i> -1 (-0.11, 0)	No phase	<i>\overline{\phi_{-1}}</i> (-6.73, 0)
TiTe <sub>2</sub>	<i>ф</i> <sub>-1</sub> (-0.93, 0)	No phase	No phase	<i>\overline{\phi_{-1}}</i> (-0.33, 0)
VOCl	<i>ф</i> -1 (-105.63, 0)	<i>ф</i> -1 (-145.87, 0)	NA	<i>φ</i> <sub>-1</sub> (-140.91, 0.14)
	<i>φ</i> <sub>-2</sub> (-154.42 0.14)			repeat of 2×2
ZrTe <sub>2</sub>	<i>ф</i> <sub>-1</sub> (-0.16, 0)	$\phi_{-1}$ (-0.53, 0)	<i>\overline{\phi_{-1}}</i> (-0.41, 0)	$\phi_{-1}$ (-0.27, 0)
	<i>\$</i> -2 (-0.82, 0)			

ZrTe <sub>3</sub>	$\phi_{-1}$ (-0.77, 0)	$\phi_{-1}$ (-1.1, 0)	NA	$\phi_{-1}$ (-0.27, 0)
	$\phi_{-2}$ (-1.39, 0)			
ZrTiSe <sub>4</sub>	<i>ф</i> -1 (-4, 0.25)	<i>ф</i> -1 (-0.14, 0)	NA	<i>φ</i> <sub>-1</sub> (-4.43, 0.25)
		$\phi_{-2}$ (-0.58, 0)		repeat of 2×2
ZrTiTe <sub>4</sub>	$\phi_{-1}$ (-4.29, 0)	<i>ф</i> <sub>-1</sub> (-0.47, 0)	NA	$\phi_{-1}$ (-4.82, 0)



**Figure S1:** Top view of TaS<sub>2</sub>-T  $3 \times 3 \phi_{-1}$ . The brown and yellow balls represent the Ta and S atoms, respectively.



**Figure S2:** Top view of TaS<sub>2</sub>-T  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S3:** Top view of TaS<sub>2</sub>-H  $3\times 3 \phi_{-1}$ .



**Figure S4:** Top view of TaS<sub>2</sub>-H 4×4  $\phi_{-1}$ .



**Figure S5:** Top view of TaSe<sub>2</sub>-T  $3\times 3 \phi_{-1}$ . The brown and green balls represent the Ta and Se atoms, respectively.



**Figure S6:** Top view of TaSe<sub>2</sub>-T  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S7:** Top view of TaSe<sub>2</sub>-T  $4 \times 4 \phi_{-1}$ .



**Figure S8:** Top view of TaSe<sub>2</sub>-H  $2 \times 2 \phi_{-1}$ .

0 0 0 0 0 b

**Figure S9:** Top view of TaSe<sub>2</sub>-H  $2 \times 2 \phi_{-2}$ .



**Figure S10:** Top view of TaSe<sub>2</sub>-H  $3 \times 3 \phi_{-1}$ .



**Figure S11:** Top view of TaSe<sub>2</sub>-H  $3 \times 3 \phi_{-2}$ .

0 10 0 0 ~~~~ 0 ~~~~ 0 b

**Figure S12:** Top view of TaSe<sub>2</sub>-H  $3 \times 3 \phi_{-3}$ .



**Figure S13:** Top view of TaTe<sub>2</sub>-H  $2 \times 2 \phi_{-1}$ . The brown and dark green balls represent the Ta and Te atoms, respectively.



**Figure S14:** Top view of TaTe<sub>2</sub>-H  $2 \times 2 \phi_{-2}$ .

**Figure S15:** Top view of TaTe<sub>2</sub>-H  $3 \times 3 \phi_{-1}$ .



**Figure S16:** Top view of TaTe<sub>2</sub>-H  $3 \times 3 \phi_{-2}$ .



**Figure S17:** Top view of TaTe<sub>2</sub>-H 4×4  $\phi_{-1}$ .



**Figure S18:** Top view of NbS<sub>2</sub>-H 2×2  $\phi_{-1}$ . The dark green and yellow balls represent the Nb and S atoms, respectively.



**Figure S19:** Top view of NbS<sub>2</sub>-H  $2 \times 2 \phi_{-2}$ .



**Figure S20:** Top view of NbS<sub>2</sub>-H  $2 \times 2 \phi_{-3}$ .



**Figure S21:** Top view of NbS<sub>2</sub>-H  $3 \times 3 \phi_{-1}$ .



**Figure S22:** Top view of NbS<sub>2</sub>-H  $3 \times 3 \phi_{-2}$ .



**Figure S23:** Top view of NbS<sub>2</sub>-T  $3 \times 3 \phi_{-1}$ .



**Figure S24:** Top view of NbS<sub>2</sub>-T  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S25:** Top view of NbS<sub>2</sub>-T  $4 \times 4 \phi_{-1}$ .



**Figure S26:** Top view of NbSe<sub>2</sub>-H  $2 \times 2 \phi_{-1}$ . The dark and light green balls represent the Nb and Se atoms, respectively.

b

**Figure S27:** Top view of NbSe<sub>2</sub>-H  $2 \times 2 \phi_{-2}$ .



**Figure S28:** Top view of NbSe<sub>2</sub>-T  $3 \times 3 \phi_{-1}$ .



**Figure S29:** Top view of NbSe<sub>2</sub>-T  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S30:** Top view of NbTe<sub>2</sub>-H  $2 \times 2 \phi_{-1}$ . The dark green and brown balls represent the Nb and Se atoms, respectively.



**Figure S31:** Top view of NbTe<sub>2</sub>-H  $3 \times 3 \phi_{-1}$ .



**Figure S32:** Top view of NbTe<sub>2</sub>-H  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S33:** Top view of NbTe<sub>2</sub>-H  $\sqrt{13} \times \sqrt{13} \phi_{-2}$ .



**Figure S34:** Top view of NbTe<sub>2</sub>-H  $4 \times 4 \phi_{-1}$ .



**Figure S35:** Top view of NbTe<sub>2</sub>-T  $3 \times 3 \phi_{-1}$ .



**Figure S36:** Top view of NbTe<sub>2</sub>-T  $3 \times 3 \phi_{-2}$ .



**Figure S37:** Top view of LaGeI  $2 \times 2 \phi_{-1}$ . The dark green, blue and purple balls represent the La, Ge, and I atoms, respectively.



**Figure S38:** Top view of TiBr<sub>2</sub> 2×2  $\phi_{-1}$ . The sky blue and brown balls represent the Ti and Br atoms, respectively.



**Figure S39:** Top view of TiBr<sub>2</sub>  $3 \times 3 \phi_{-1}$ .



**Figure S40:** Top view of TiBr<sub>2</sub>  $3 \times 3 \phi_{-2}$ .



**Figure S41:** Top view of TiBr<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S42:** Top view of TiCl<sub>2</sub>  $3 \times 3 \phi_{-1}$ . The sky blue and green balls represent the Ti and Cl atoms, respectively.



**Figure S43:** Top view of TiCl<sub>2</sub>  $3 \times 3 \phi_{-2}$ . The sky blue and green balls represent the Ti and Cl atoms, respectively.



**Figure S44:** Top view of TiOBr  $2 \times 2 \phi_{-1}$ . The sky blue, red, and brown balls represent the Ti, O, and Br atoms, respectively.



**Figure S45:** Top view of TiOBr  $2 \times 2 \phi_{-2}$ .



**Figure S46:** Top view of TiOBr  $3 \times 3 \phi_{-1}$ .



**Figure S47:** Top view of TiOBr  $4 \times 4 \phi_{-1}$ .



**Figure S48:** Top view of TiOCl  $3\times 3 \phi_{-1}$ . The sky blue, red, and green balls represent the Ti, O, and Cl atoms, respectively.



**Figure S49:** Top view of TiOCl  $4 \times 4 \phi_{-1}$ .



**Figure S50:** Top view of TiS<sub>2</sub>  $2 \times 2 \phi_{-1}$ . The sky blue and yellow balls represent the Ti and S atoms, respectively.



**Figure S51:** Top view of TiS<sub>2</sub>  $3 \times 3 \phi_{-1}$ .



**Figure S52:** Top view of TiSe<sub>2</sub>  $3 \times 3 \phi_{-1}$ . The sky blue and light green balls represent the Ti and Se atoms, respectively.



**Figure S53:** Top view of VOCl  $2 \times 2 \phi_{-1}$ . The royal blue, red, and light green balls represent the V, O, and Cl atoms, respectively.



**Figure S54:** Top view of VOCl  $2 \times 2 \phi_{-2}$ .



**Figure S55:** Top view of VOCl  $3 \times 3 \phi_{-1}$ .



**Figure S56:** Top view of  $ZrTe_2 2 \times 2 \phi_{-1}$ . The orange and green balls represent the Zr and Te atoms, respectively.



**Figure S57:** Top view of ZrTe<sub>2</sub>  $2 \times 2 \phi_{-2}$ .



**Figure S58:** Top view of ZrTe<sub>3</sub>  $2 \times 2 \phi_{-1}$ . The same color convention of the last 2 Figures has been used.



**Figure S59:** Top view of ZrTe<sub>3</sub>  $2 \times 2 \phi_{-2}$ .



**Figure S60:** Top view of  $ZrTe_3 3 \times 3 \phi_{-1}$ .



**Figure S61:** Top view of ZrTiSe<sub>4</sub>  $3 \times 3 \phi_{-1}$ . The orange, blue, and green balls represent the Zr, Ti and Se atoms, respectively.



**Figure S62:** Top view of ZrTiSe<sub>4</sub>  $3 \times 3 \phi_{-2}$ .



**Figure S63:** Band structure of  $1\text{T-TaS}_2 \sqrt{13} \times \sqrt{13} \phi_{-2}$  (CCDW). Note that for this and all subsequent band structures, the supercell band structure is presented and thus, the effect of BZ folding is included.



**Figure S64:** Band structure of 1T-TaSe<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S65:** Band structure of 1T-NbSe<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S66:** Band structure of 2H-NbTe<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S67:** Band structure of 2H-NbTe<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-2}$ .



**Figure S68:** Band structure of TiBr<sub>2</sub>  $2 \times 2 \phi_{-1}$ .



**Figure S69:** Band structure of TiBr<sub>2</sub>  $3 \times 3 \phi_{-2}$ .



**Figure S70:** Band structure of TiBr<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S71:** Band structure of TiCl<sub>2</sub>  $2 \times 2 \phi_{-1}$ .



**Figure S72:** Band structure of TiCl<sub>2</sub>  $3 \times 3 \phi_{-2}$ .



**Figure S73:** Band structure of TiCl<sub>2</sub>  $\sqrt{13} \times \sqrt{13} \phi_{-1}$ .



**Figure S74:** Band structure of TiOCl  $4 \times 4 \phi_{-1}$ .



**Figure S75:** Band structure of TiS<sub>2</sub>  $2 \times 2 \phi_{-1}$ .



**Figure S76:** Band structure of TiS<sub>2</sub>  $3 \times 3 \phi_{-1}$ .



**Figure S77:** Band structure of VOCl  $2 \times 2 \phi_{-2}$ .



**Figure S78:** Band structure of ZrTiSe<sub>4</sub>  $2 \times 2 \phi_{-1}$ .

## **Computational Methods**

DFT calculations are carried out using the generalized gradient approximation(GGA) as implemented in the code VASP<sup>1-4</sup> with the PAW<sup>5</sup> method using the Perdew–Burke–Ernzenhof (PBE)<sup>6</sup> exchange-correlation functional. The pseudopotentials recommended by VASP have been used throughout. Sufficiently large cutoff energy of 550 eV is used to avoid any Pulay stress. For all structural relaxations,  $a > \frac{30}{a} \times \frac{30}{b} \times 1$  Gamma-centered *k*-points grid is used to sample the Brillouin zone, where *a* and *b* are the lattice parameters of the particular supercell. A >  $\frac{60}{a} \times \frac{60}{b} \times 1$  similar *k*-mesh is used for all static runs. The charge densities generated by these static runs have been used to perform the non-self-consistent band structure runs. Electronic convergence is set to be attained when the difference in energy of successive electronic steps becomes less than  $10^{-6} \text{ eV}$ , whereas the structural geometry is optimized until the maximum Hellmann–Feynman force on every atom falls below 0.01 eV/Å. A large vacuum space of  $\geq 25$  Å in the direction of **c** is applied to avoid any spurious interaction between periodically repeated layers.

For the ZrTiSe<sub>4</sub> Fermi surface calculation, the code QuantumATK<sup>7</sup> has been used in conjunction with the PBE functional, where the accuracy of the calculations mostly depends on the selection of norm-conserving pseudopotentials and numerical LCAO basis sets. The "SG15" norm-conserving pseudopotentials with "Medium" basis sets have been used. The optimized "SG15" provides smooth pseudopotentials with multiple projectors and non-linear core corrections<sup>8,9</sup>. A  $7 \times 13 \times 1$  *k*-points sampling and cutoff energy of 75 Hartree has been employed for both structural relaxation, and band structure/Fermi-surface calculation. The obtained relaxed crystal and band structure is found to be almost identical to those produced by VASP, establishing transferability of the results across different DFT codes and methods.

Phonon calculations are done using the code Phonopy<sup>10</sup>, which uses the atomic forces calculated by VASP based on finite displacement method applied to 2×2 magnified cells employing a >  $\frac{60}{a} \times \frac{60}{b} \times 1$  *k*-mesh and 10<sup>-8</sup> eV electronic convergence criteria.

The "Shake & Relax" protocol of the package AIRSS<sup>11</sup> interfaced with VASP has been used to produce the distorted structures. A minimum separation of 2 Å is kept between all atoms to minimize unphysical atomic overlaps. The same rigorous DFT relaxation criteria mentioned before

have been implemented here. The AIRSS Shake & Relax algorithm and its highly parallel masterslave implementation are similar to that of our previous works<sup>12,13</sup>. To accelerate the DFT calculations, hardware-accelerators have been employed extensively. GPU version of VASP code<sup>14,15</sup> is used, and regular CPU code is adapted for execution in Xeon-Phi (KNL)<sup>16</sup>.

To generate inputs, parse outputs and measure the RMS displacements, which have been taken as the measure of distortion, the package pymatgen<sup>17</sup> is employed. The "Mean-shift" algorithm as implemented in the package scikit-learn<sup>18</sup> is used to perform the unsupervised clustering. The bandwidth for the clustering process has been obtained with the "estimate\_bandwidth" function which takes two inputs, the data-set and a quantile value (0.3-0.45). The band structure unfolding has been performed with the tool vaspkit<sup>19</sup> interfaced with VASP. All crystal-structure images are generated using the tool VESTA<sup>20</sup>.

All CDW crystal structure files (cif) and their top-view images (png) are available at the OSF repository. (<u>https://osf.io/by7et</u>).

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