Ab Initio Study of Mismatched Layered Superconductors

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PARADIM — AN NSF MATERIALS INNOVATION PLATFORM

Bardeen-Cooper-Schrieffer Theory

$$k_B T_c = 1.135\, E_D e^{\frac{-1}{N(0)\,V}}$$

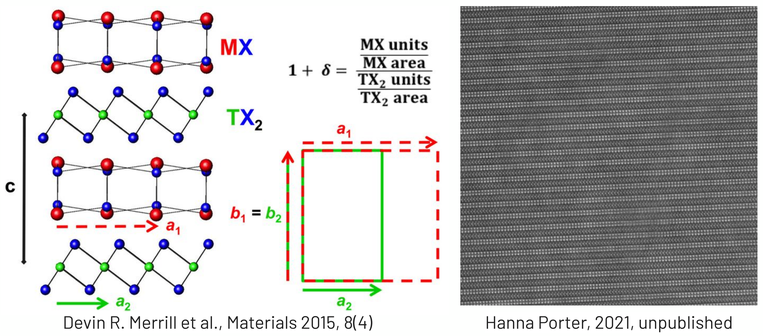
- T_c - superconducting transition temperature
- E_D - Debye energy (not exponentially sensitive)
- V - electron-phonon coupling (shouldn't vary much within a column of periodic table)
- $N(0)$ - electron density of states at Fermi level, evaluated using density-functional theory (DFT)

Mismatched Layered Materials

- consist of 2 alternating layers: a rocksalt and a transition metal dichalcogenide (TMD)
- defined by the formula BiX + NbY_2, where X is S, Se, or Te and Y is S, Se, creating the following materials:

		rock salt		
		BiS	BiSe	BiTe
TMD	NbS_2	BiS + NbS_2	BiSe + NbS_2	BiTe + NbS_2
	$NbSe_2$	BiS + $NbSe_2$	BiSe + $NbSe_2$	BiTe + $NbSe_2$

Incommensurate Lattices

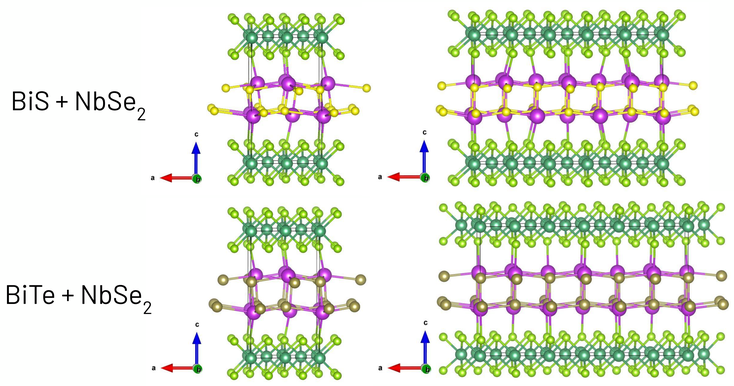


Devin R. Merrill et al., Materials 2015, 8(4)

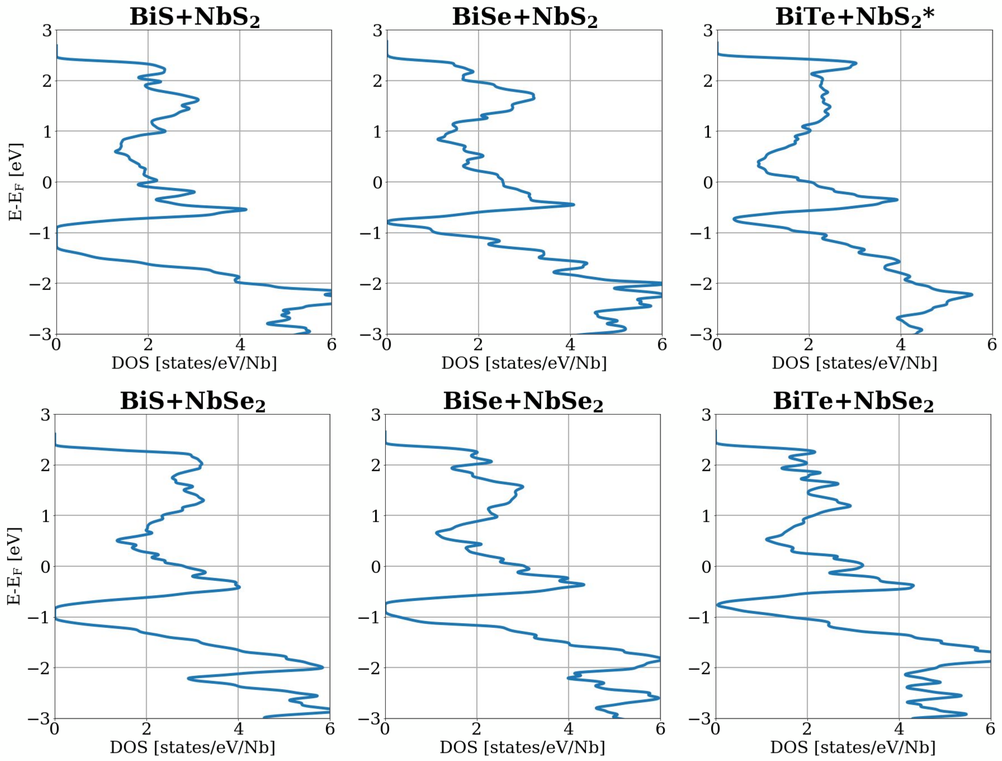
Hanna Porter, 2021, unpublished

- rational number approximations (rocksalt:TMD)

	BiS		BiSe		BiTe	
	1 + δ	rs : TMD	1 + δ	rs : TMD	1 + δ	rs : TMD
NbS_2	1.109	10:9	1.034	1:1	0.930	13:14
$NbSe_2$	1.194	6:5	1.110	10:9	1.001	1:1



Density of States (DOS)



Fermi Level Density of States

[states/eV/Nb]	BiS	BiSe	BiTe
NbS_2	2.1	2.5	2.0*
$NbSe_2$	2.8	3.0	3.2

T_c Enhancements

- T_c for monolayer NbS_2 and monolayer $NbSe_2$ are 1.8 K and 3.1 K respectively. Listed below are the factors by which the superconducting temperature of each material improved compared to their respective monolayer TMD:

	BiS	BiSe	BiTe
NbS_2	5.0	9.3	4.6*
$NbSe_2$	6.8	8.1	8.9

*results for BiTe+NbS_2 are preliminary

Conclusions:

The density of states calculations indicate that BiTe+$NbSe_2$ has the highest density of states at the Fermi level for this particular family of materials. Furthermore, this material is suspected to have the greatest T_c enhancement. Since T_c for monolayer $NbSe_2$ is 3.1K and the calculated enhancement is a factor of 8.88, we hypothesize that T_c for BiTe+$NbSe_2$ could be as high as 27 K.

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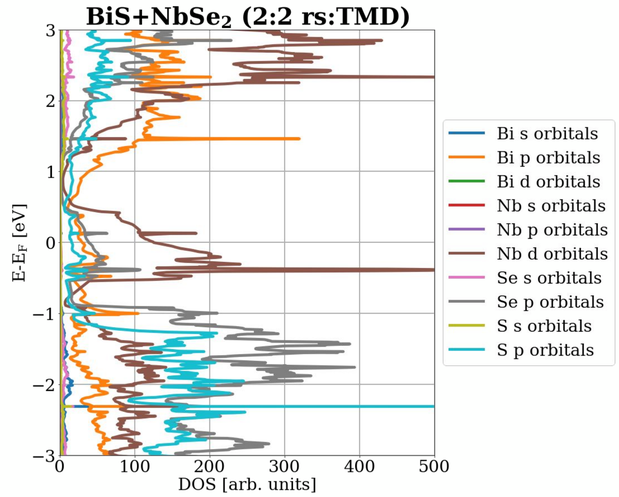
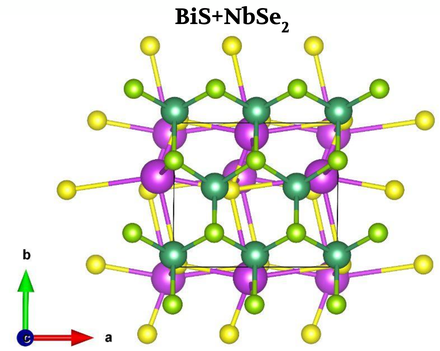
Projected Density of States (PDOS)



- The largest contributions to the DOS at the Fermi level come from the *d* orbitals of the Nb atoms. The PDOS results for the other materials support this as well.

Lattice Constants



- lattice constants increase as elements in TMD layer and elements in rocksalt layer increase in size

[Å]	BiS			BiSe			BiTe		
	a	*b*	*c*	*a*	*b*	*c*	*a*	*b*	*c*
NbS_2	6.61	5.76	11.60	6.58	5.82	11.80	6.62	6.00	12.09
$NbSe_2$	6.87	6.04	12.29	6.90	6.06	12.39	6.81	6.15	12.57

Why is Bigger Better?

As larger X and Y atoms are used in the layered material, the designated by the *a* and *b* lattice vectors increases. These areas are listed in the table below. As a result of the increased lattice size, atoms in the material are spread out more, increasing the number of states in a given energy range. Thus, the resulting trend indicates that materials with larger lattice constants have a higher DOS at the Fermi level.

$a \times b$ [Å^2]	BiS	BiSe	BiTe
NbS_2	38.08	38.29	39.73
$NbSe_2$	41.51	41.80	41.89