MECHANICAL STABILITY AND ELECTRONIC PROPERTIES OF HETEROSTRUCTURES BASED ON β-InSe / $MoSe_2$

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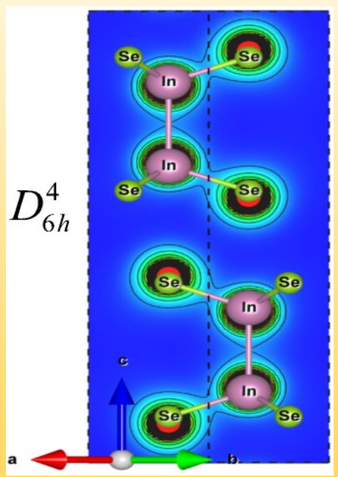
Abstract

As is known, the crystal β-InSe is characterized by its layered structure and unique electronic properties, making it quite valuable for applications in electronics and optoelectronics. On the other hand, $MoSe_2$, is also a material with a quasi-two-dimensional structure, which has a wide range of potential applications, especially in the field of semiconductor devices and photodetectors. Consequently, studying the electronic properties of the created heterostructures β-InSe/$MoSe_2$ is of interest. Particularly relevant is the question of their mechanical stability, as only mechanically stable heterostructures can open up new opportunities for the development and optimization of devices based on such materials.

This study investigates the electronic properties and mechanical stability of proposed two models of heterostructures formed by the combination of two quasi-two-dimensional materials: β-InSe and $MoSe_2$. Using computational methods, we showed that both models of β-InSe/$MoSe_2$ heterostructures exhibit similar electronic band structures, with indirect bandgaps and overlapping states between the conduction and valence bands. Mechanical properties were also analyzed, revealing that both heterostructure models are mechanically stable. However, one model showed lower anisotropy and higher stability offering potential for future applications in advanced physics technologies.

Energy bands structure of the β-InSe crystal

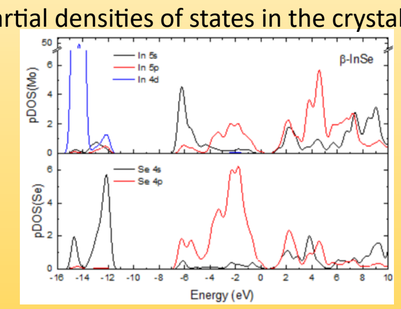
Lattice parameters are equal: a=b=4.05 A^0, c=16.930 A^0



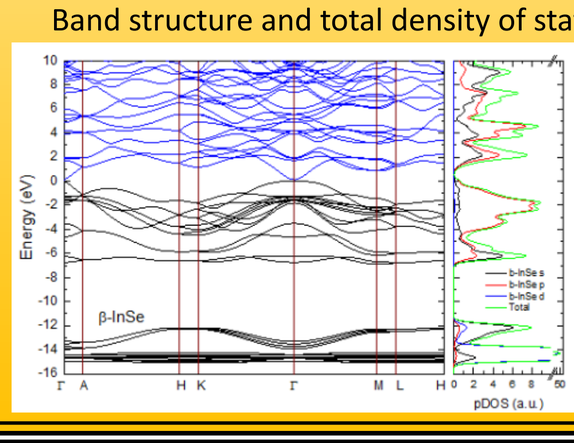
Relative coordinates of β-InSe atoms

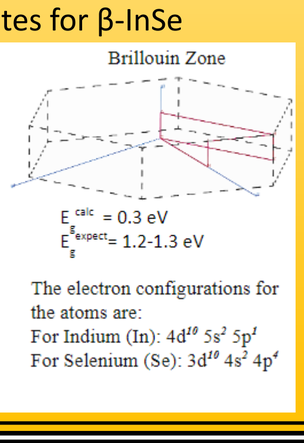
Atom	X	Y	Z	Position
Se	0.33333	0.66667	0.89800	4f
In	0.33333	0.66667	0.15700	4f

Partial densities of states in the crystal β-InSe



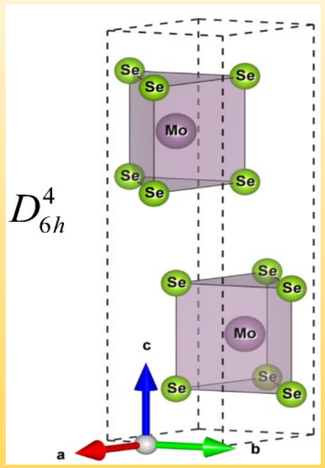
Band structure and total density of states for β-InSe





Energy bands structure of the $MoSe_2$ crystal

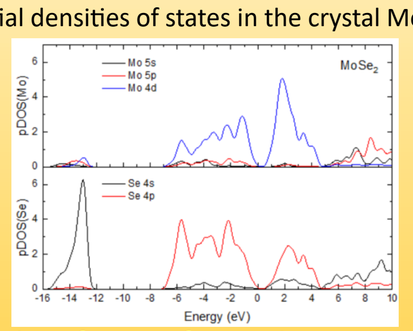
Lattice parameters are equal: a=b=3.289 A^0, c=12.927 A^0



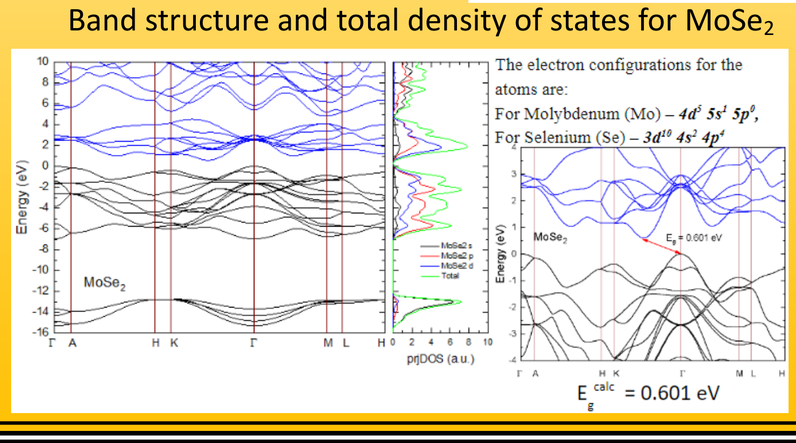
Relative coordinates of $MoSe_2$ atoms

Atom	X	Y	Z	Position
Se	0.33333	0.66667	0.62100	4f
Mo	0.33333	0.66667	0.25000	2c

Partial densities of states in the crystal $MoSe_2$

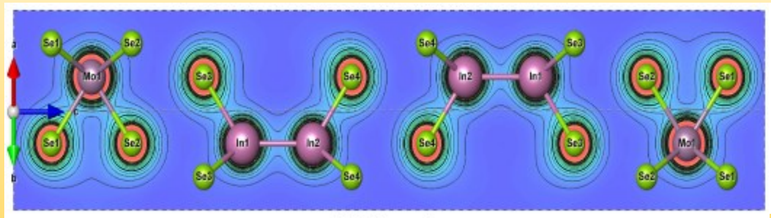


Band structure and total density of states for $MoSe_2$



MODELING OF THE HETEROSTRUCTURES BASED ON β-InSe / $MoSe_2$

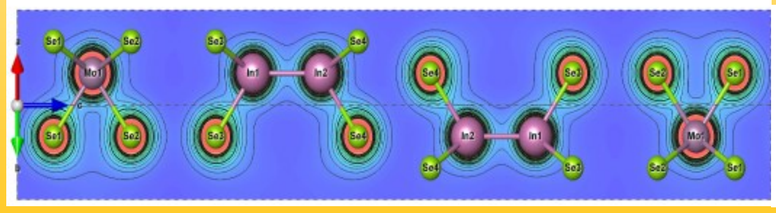
Elementary cell of the β-InSe/$MoSe_2$ heterostructure and spatial distribution of the electronic density



P-3m1

Model 1

$a=b$=3.57737 A°,
c= 29.03070 A°,
α=β=90.00°
γ= 120.00 °

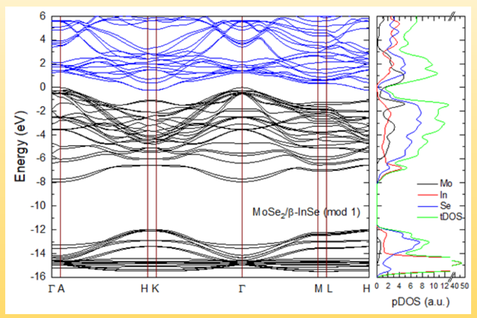


Model 2

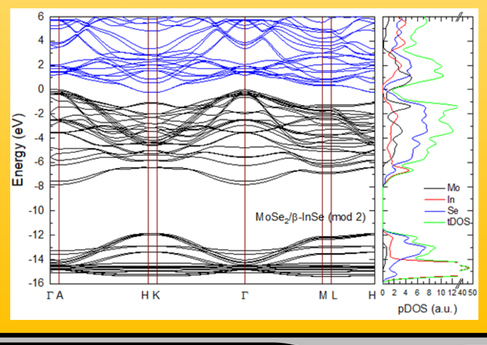
a=b=3.66950 A°,
c= 29.85700A°,
α=β=90.00°,
γ= 120.00°

These heterostructures consist of two sets of translationally inequivalent layers: Se–Mo–Se and Se-In-In-Se structures, which are positioned perpendicular to the hexagonal axis 0z.

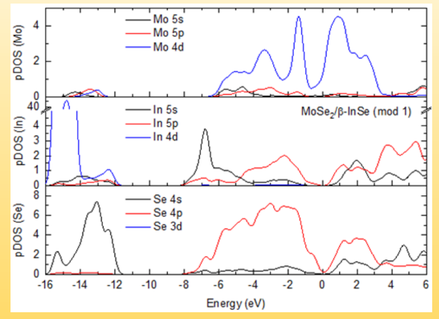
Band structure of the β-InSe/$MoSe_2$ heterostructure for Model 1



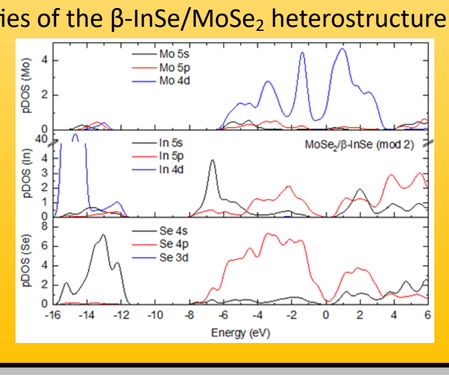
Band structure of the β-InSe/$MoSe_2$ heterostructure for Model 2



Partial densities of the β-InSe/$MoSe_2$ heterostructure for Model 1



Partial densities of the β-InSe/$MoSe_2$ heterostructure for Model 2



Elastic properties for crystals of β-InSe and $MoSe_2$, *and heterostructures* β-InSe/$MoSe_2$

Parameters	β -InSe	$MoSe_2$	β-InSe/$MoSe_2$ (model 1)	β InSe/$MoSe_2$ (model 2)
Average sound velocity, (m/s)	1967.15637	2840.73943	2118.59962	1485.04842
Bulk modulus, B (GPa)	37.56016 +/- 1.176	54.91150 +/- 0.777	42.37027 +/- 0.614	36.02267 +/- 2.504
Shear modulus G (GPa)	18.96337	57.86705	27.31181	22.33745
B/G ratio	1.98	0.95	1.55	1.61
Generalized anisotropy parameter	0.39	1.28	1.07	9.46
C_{11}, GPa	70.58870 +/- 0.577	205.89515 +/- 1.740	110.54075 +/- 0.101	105.18155 +/- 1.297
C_{12}, GPa	24.31135 +/- 2.612	46.54750 +/- 0.468	41.83660 +/- 1.709	39.15100 +/- 2.929
C_{13}, GPa	21.71788 +/- 1.700	13.18543 +/- 0.819	15.19655 +/- 0.256	7.66660 +/- 5.001
C_{14}, GPa			-1.15200 +/- 1.868	-0.23110 +/- 0.700
C_{15}, GPa			0.00000 +/- 0.000	0.00000 +/- 0.000
C_{33}, GPa	62.93740 +/- 5.114	79.32700 +/- 1.688	64.20485 +/- 1.910	58.26910 +/- 1.122
C_{44}, GPa	13.11115 +/- 2.282	35.13090 +/- 2.198	15.59405 +/- 0.113	3.64465 +/- 0.769
C_{66}, GPa	23.14	79.76	34.35	33.02
E_{xy}	0.2665	0.2177	0.3586	0.3663
E_xz	0.2531	0.1300	0.1518	0.0834
E_{yx}	0.2665	0.2177	0.3586	0.3663
E_{yz}	0.2531	0.1300	0.1518	0.0834
E_{zx}	0.2289	0.0522	0.0997	0.0531
E_{zy}	0.2289	0.0522	0.0997	0.0531
Young's Modulus X	58.61206	194.04515	93.11361	90.17991
Young's Modulus Y	58.61206	194.04515	93.11361	90.17991
Young's Modulus Z	52.99712	77.94961	61.17375	57.45464

The reduced parameter of generalized anisotropy for the heterostructure - InSe/$MoSe_2$ in model 1 indicates a lower anisotropy of properties in this heterostructure.

$C_{13(m1)}$ / $C_{13(m2)}$ ~ 2 and $C_{44(m1)}$ / $C_{44(m2)}$ ~ 4.3 indicate a stronger interlayer coupling in the heterostructure β-InSe/$MoSe_2$ model 1.

The estimates of the final enthalpy:
E_{model1} = -3.817**35**729E+004 eV
E_{model2} = -3.817**33**376E+004 eV

indicate a higher energetic stability for the β-InSe/$MoSe_2$ heterostructure for Model 1.

Evaluation of the Born criterion

Born Criterion	β -InSe	$MoSe_2$	β-InSe/$MoSe_2$ (model 1)	β-InSe/$MoSe_2$ (model 2)
$\frac{C_{11}}{\lvert C_{12}\rvert}$	2.9	4.42	2.64	2.68
$\frac{2C_{13}^2}{C_{33}(C_{11}+C_{12})}$	0.16	0.019	0.04	0.014

The obtained data indicate that the Born criterion conditions are met; therefore, all structures are mechanically stable. However, considering the anisotropy parameter, minimal energy, and changes in interlayer bonding, we conclude that model 1 of the β-InSe/$MoSe_2$ heterostructure is energetically more favorable.

Conclusion:

Energy spectra, spatial distribution of valence electrons, and Mulliken charges were investigated for bulk crystals of β-InSe and $MoSe_2$, as well as for heterostructures based on them. For both models of the heterostructures, the band gap remains indirect, with the displacement of the main conduction band extremum to the high-symmetry K point of the Brillouin zone for hexagonal symmetry, and there is also a decrease compared to Eg for β-InSe and $MoSe_2$ crystals, down to the overlapping of the bottom of the conduction band and the top of the valence band. It has been shown that there is no significant difference in the formation of valence band states for the two models of the considered heterostructures.

Mechanical characteristics (elastic moduli, Young's moduli, Poisson's ratios) were calculated for bulk crystals of β-InSe and $MoSe_2$, as well as for InSe/$MoSe_2$ heterostructures. It was found that the elastic constants C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66} for both models of the heterostructures are almost identical in numerical value, except for the elastic constants C_{13} and C_{44}, which characterize the interlayer bonding. Both β-InSe/$MoSe_2$ heterostructures were determined to be mechanically stable based on the Born criterion assessment.

The reduced parameter of generalized anisotropy for the β-InSe/$MoSe_2$ heterostructure in model 1 (1.07) indicates lower anisotropy of properties in this heterostructure. Minimal energy and interlayer bonding also confirm the higher stability of this model 1.

Therefore, based on the above results, it can be concluded that the β-InSe/$MoSe_2$ heterostructure in model 1 proved to be more mechanically stable and energetically favorable, making it promising for further research and potential use in high-tech applications in physics.