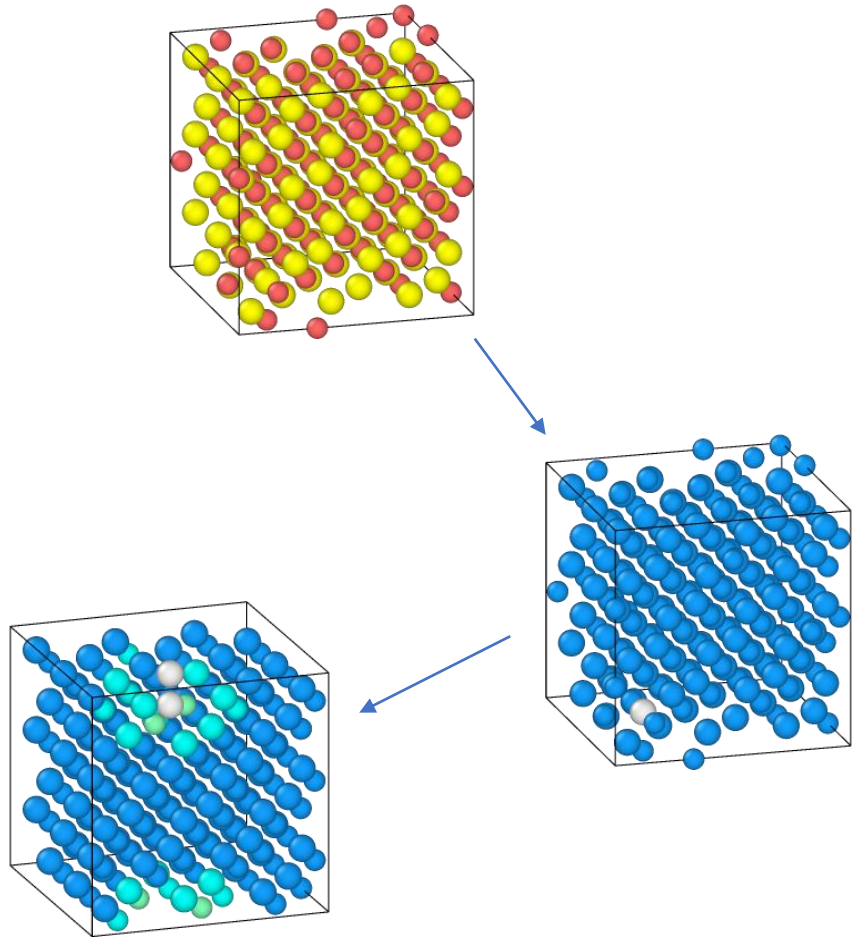
Activation barriers for the diffusion of Se interstitials in CdTe and CdSe



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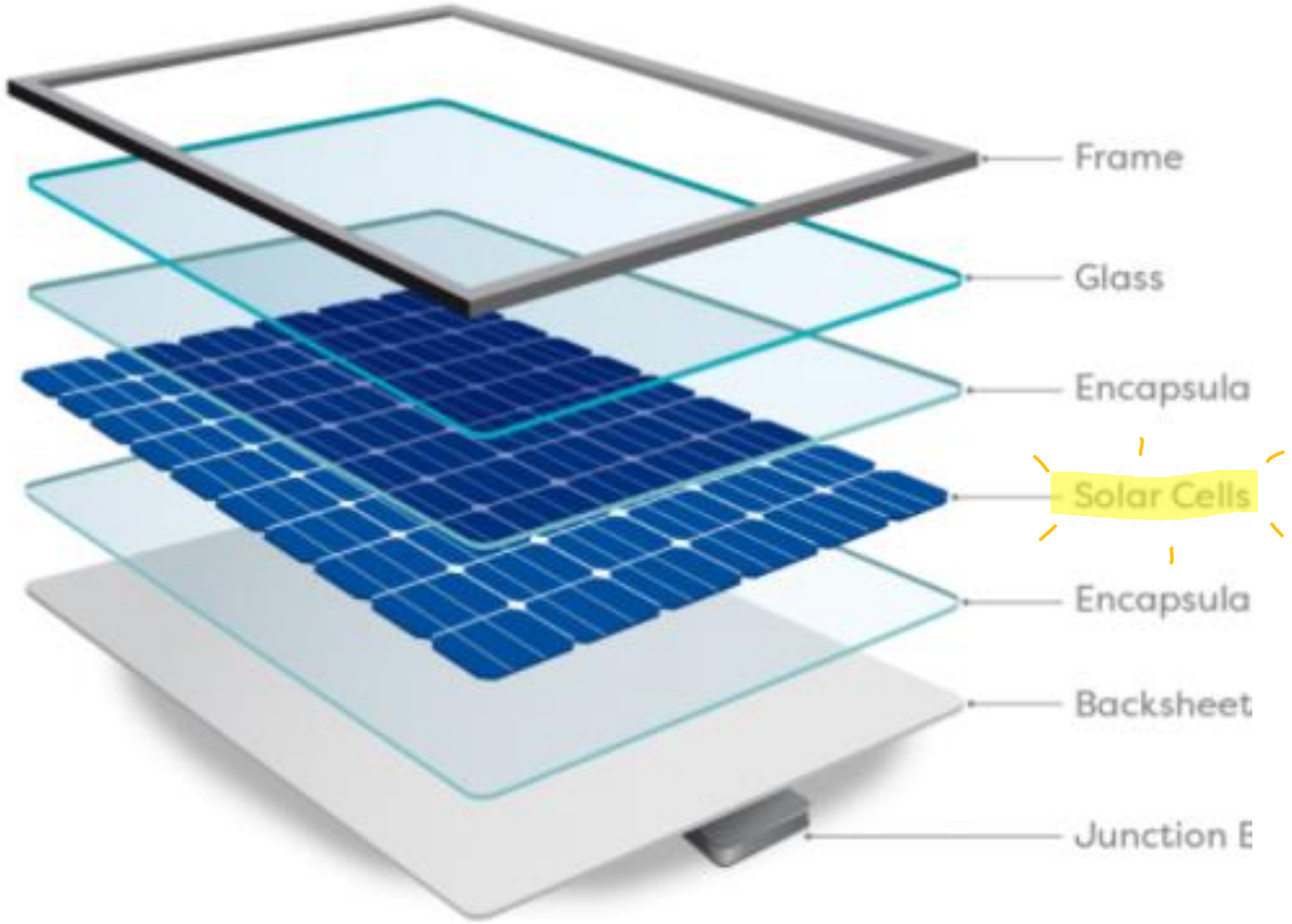
Special thanks to: Indiras khatri, Sameer hamadna
Prof. Michael Heben

Introduction

Learning about molecular Dynamics (MD) and solar cells.

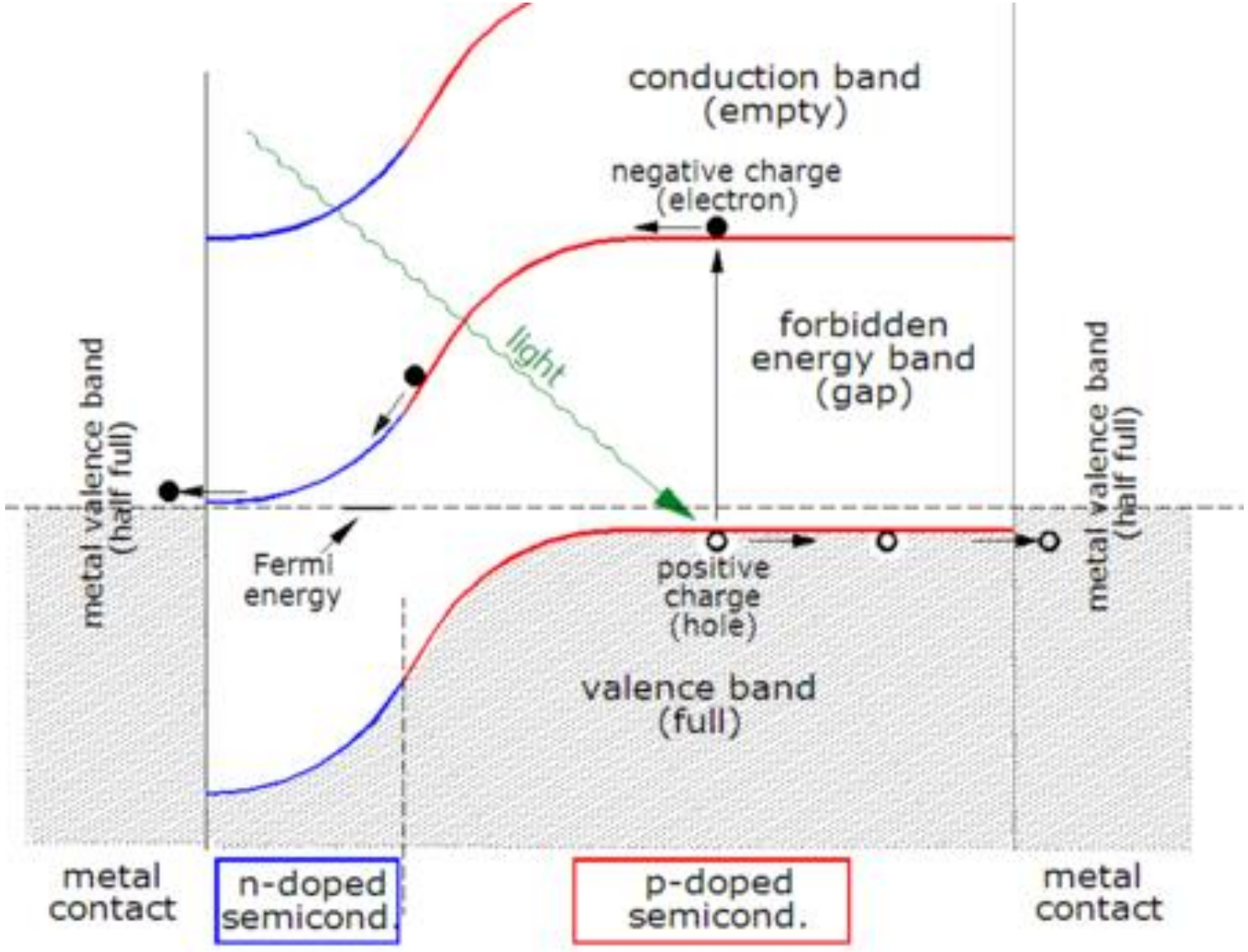
The Solar Cell

A solar panel is made up of many parts, but for our research, we are focused specifically on the solar cell. This part of the solar panel is in charge of producing electricity from light. Solar cells can also be made from thin film material.

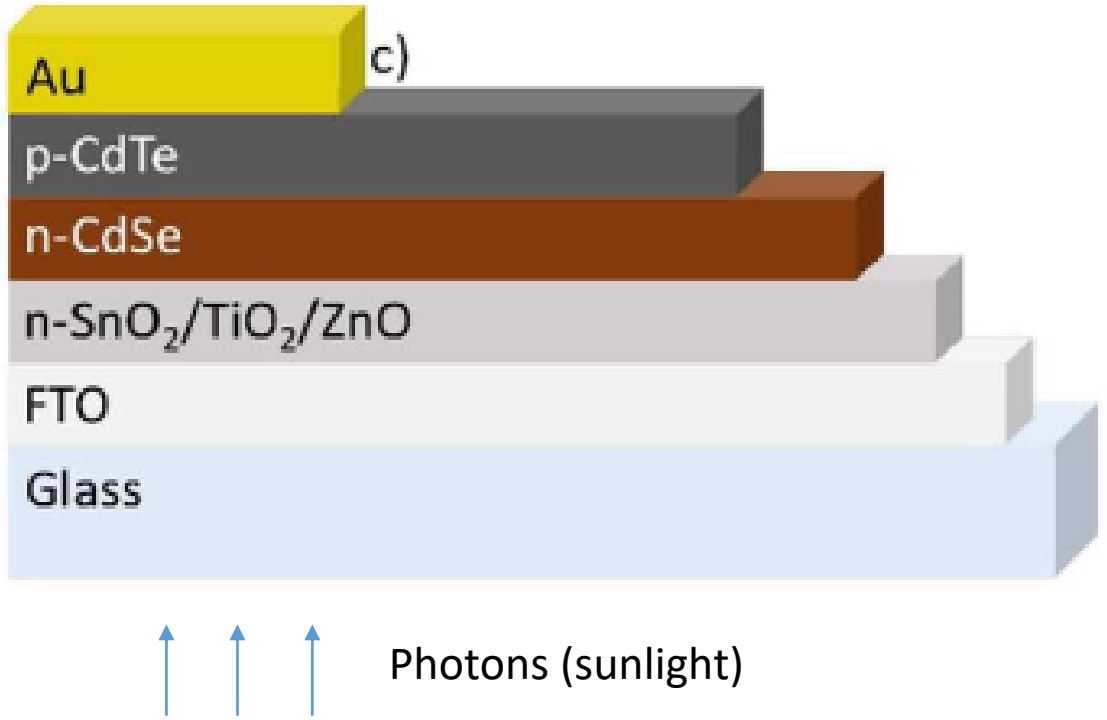


Light Into Electricity

For a photon to be absorbed by an electron in the semiconductor (CdTe). The photon energy must be greater than the energy band gap. The electron is then excited and jumps to the empty conduction band, leaving a hole in the valence band. After this, the electron (hole) are free to move around in the conduction band (valence band) generating current!



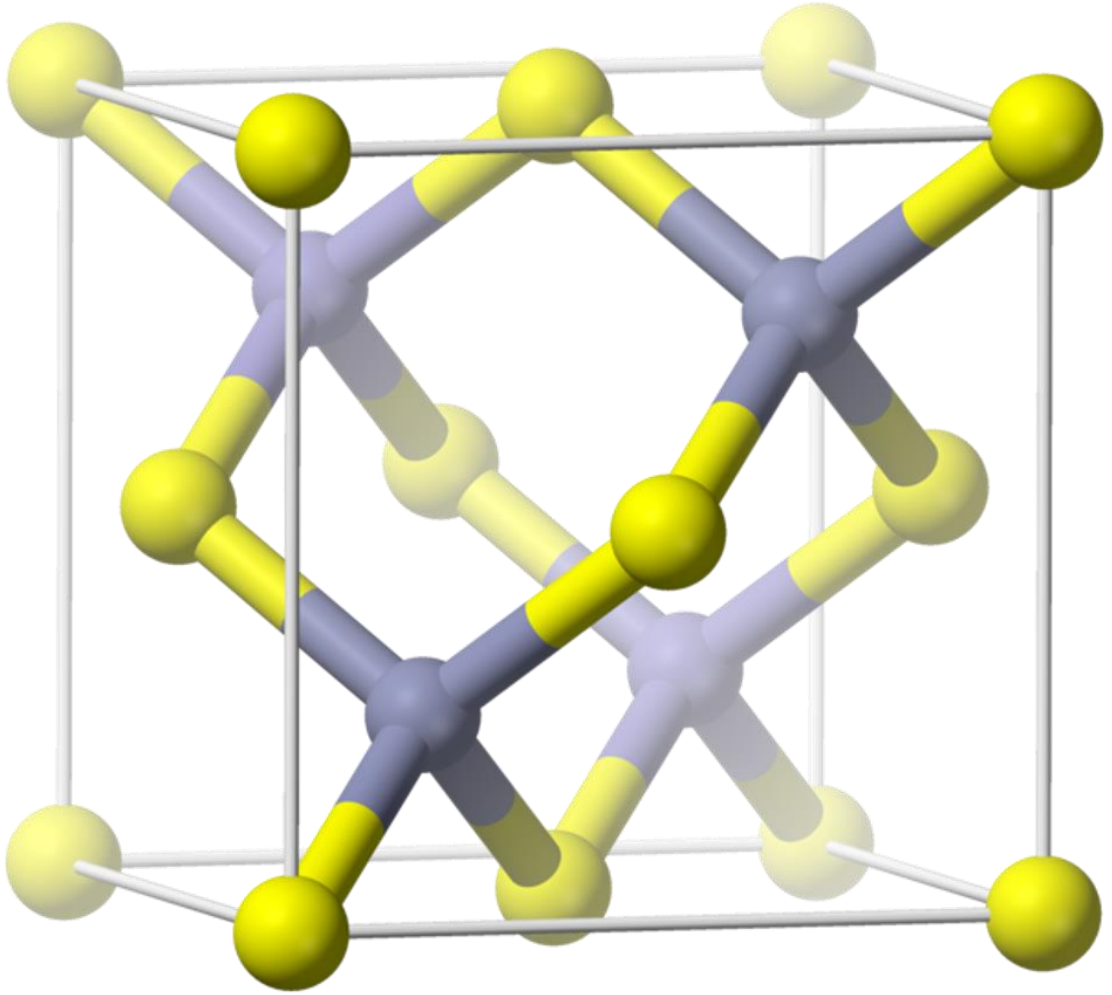
CdTe/CdSe Solar Cell about MD and solar cells.



Example of CdTe / CdSe solar cell: *Solar Energy Materials and Solar Cells 180 (2018) 196-204*

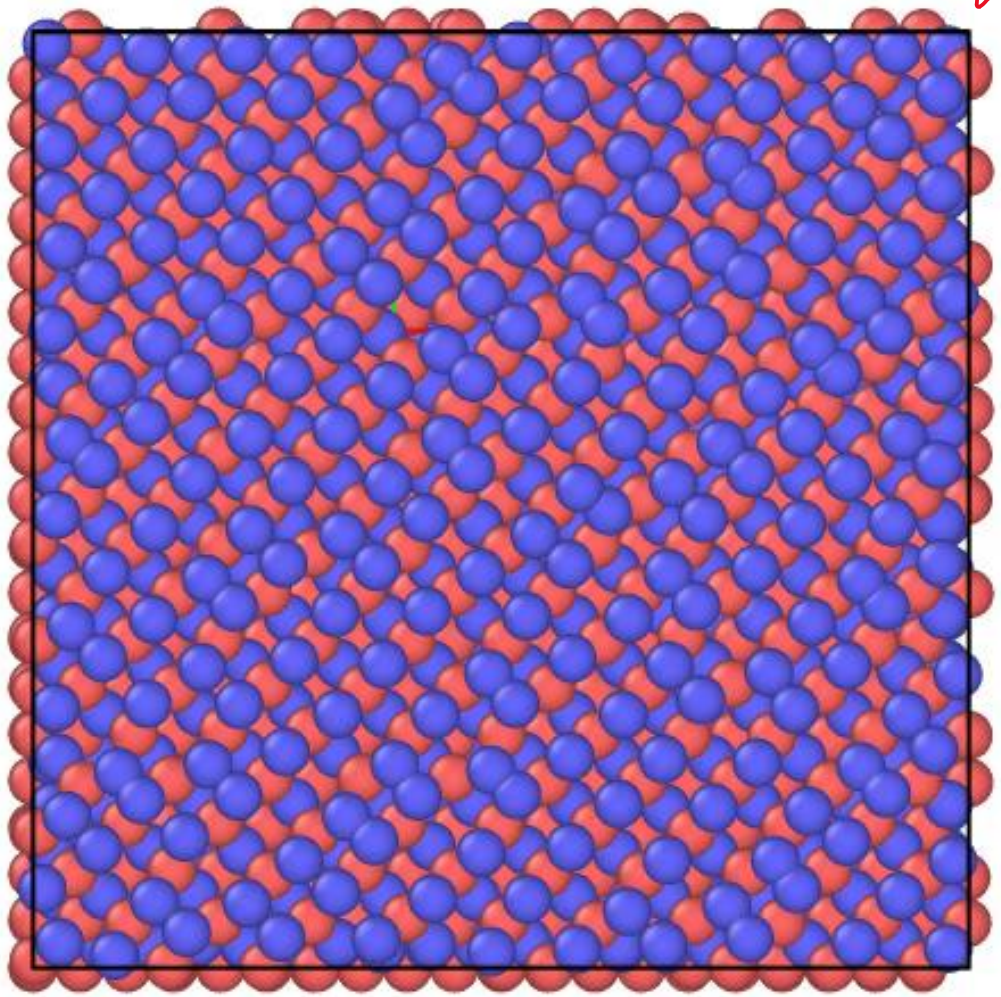
CdTe/CdSe crystal structure

Both CdTe and CdSe have the zincblende structure corresponding to two interpenetrating face centered cubic (fcc) lattices.



What is MD?

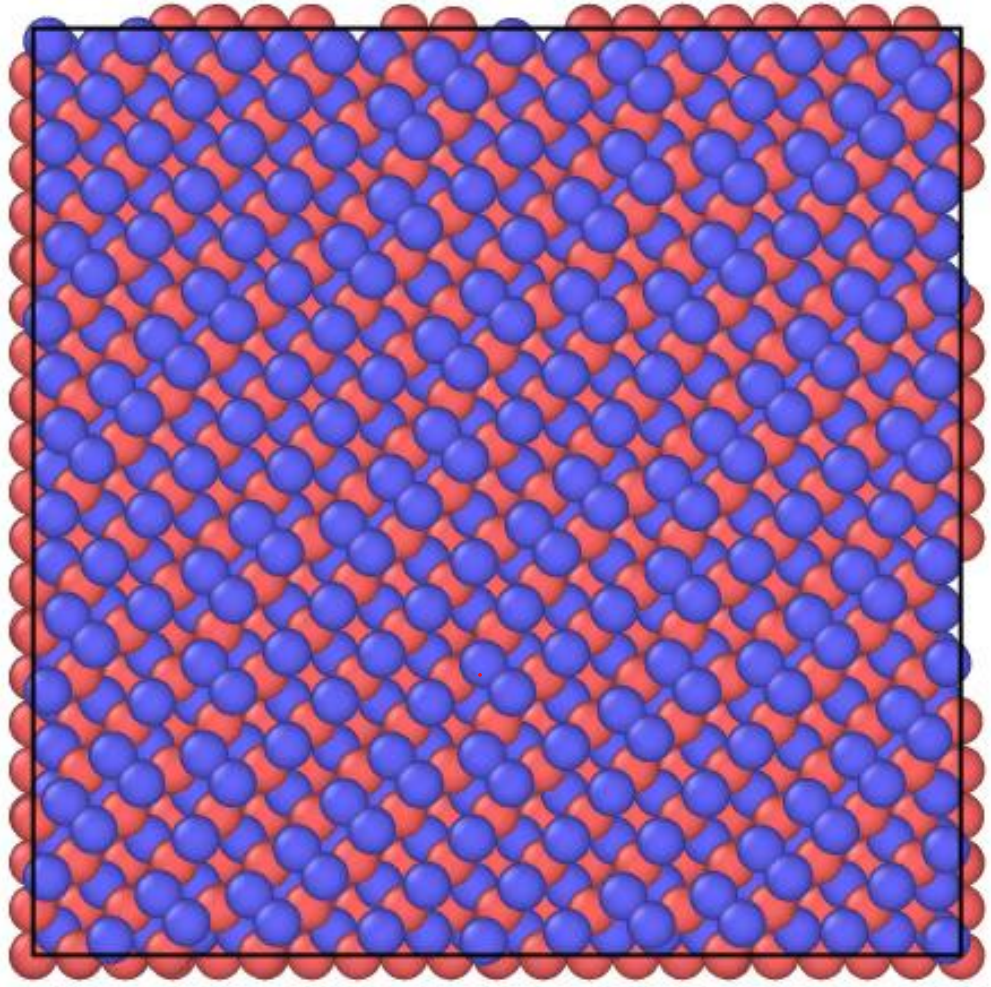
MD stands for molecular dynamics which is a computer simulation method for simulating the motion of atoms and molecules on short (ns-ms) time scales. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic evolution of the system.



CdTe (100) surface

Movie of minimized snap shots of CdTe(100) surface showing transitions

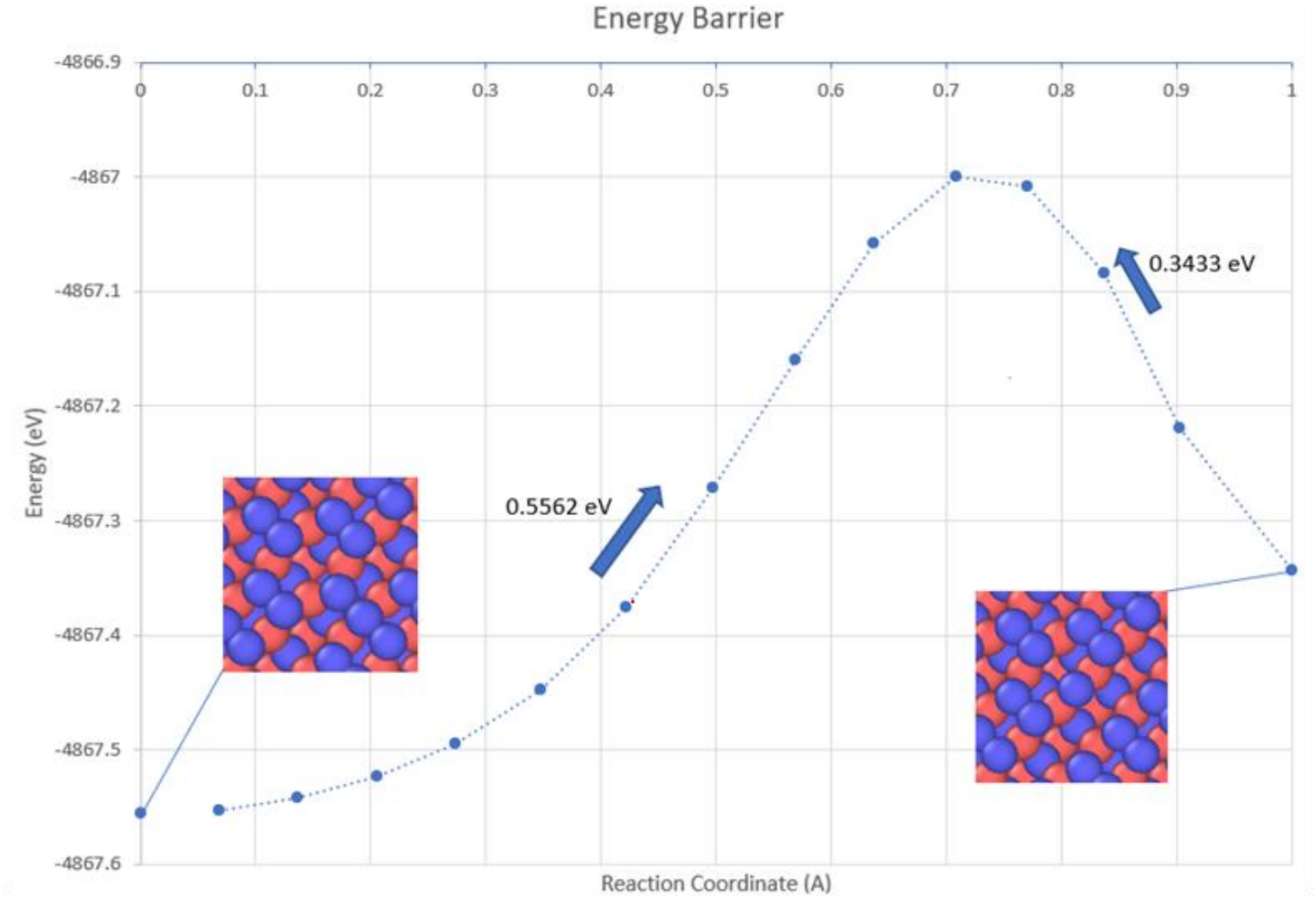
Minimization is the process of changing the force acting on each atom acceptably close to zero causing the position to be more stable. In return this makes the simulation more readable.



CdTe (100) surface

Finding the energy barrier for transitions using the nudged elastic band (NEB) method

This method finds the minimum energy path between two minimized states as well as the energy barrier (saddle point) corresponding to the peak along the path.

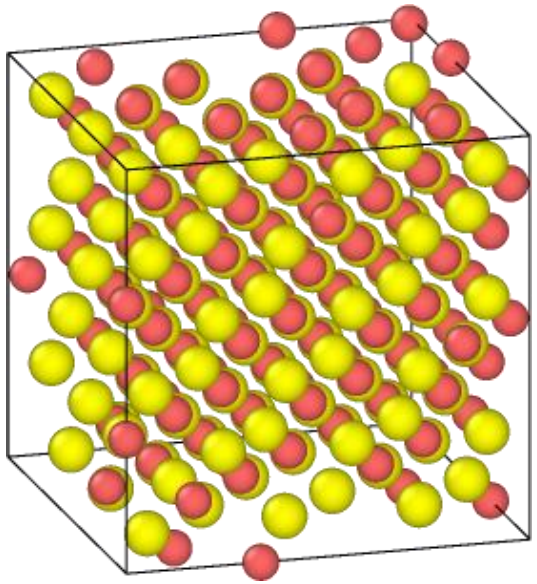


Diffusion of Se interstitials in CdTe and CdSe

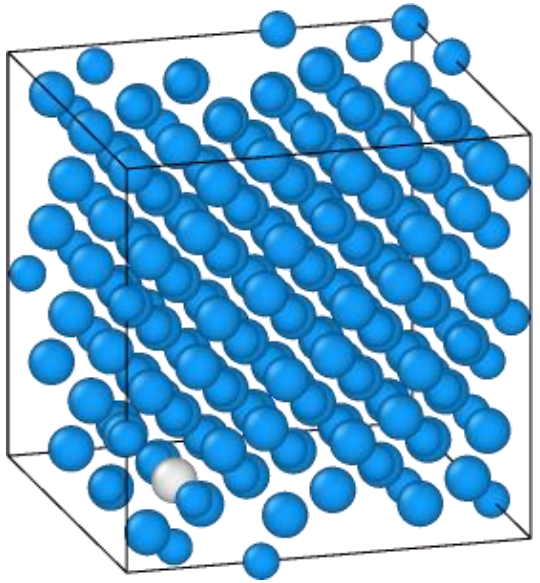
Applying what I learned.

Se interstitial in CdSe: initial configuration

An initial configuration was set and over time the simulation went on evolving from there. However, to find the interstitial we had to alter the visuals of the simulation (as seen to the right).

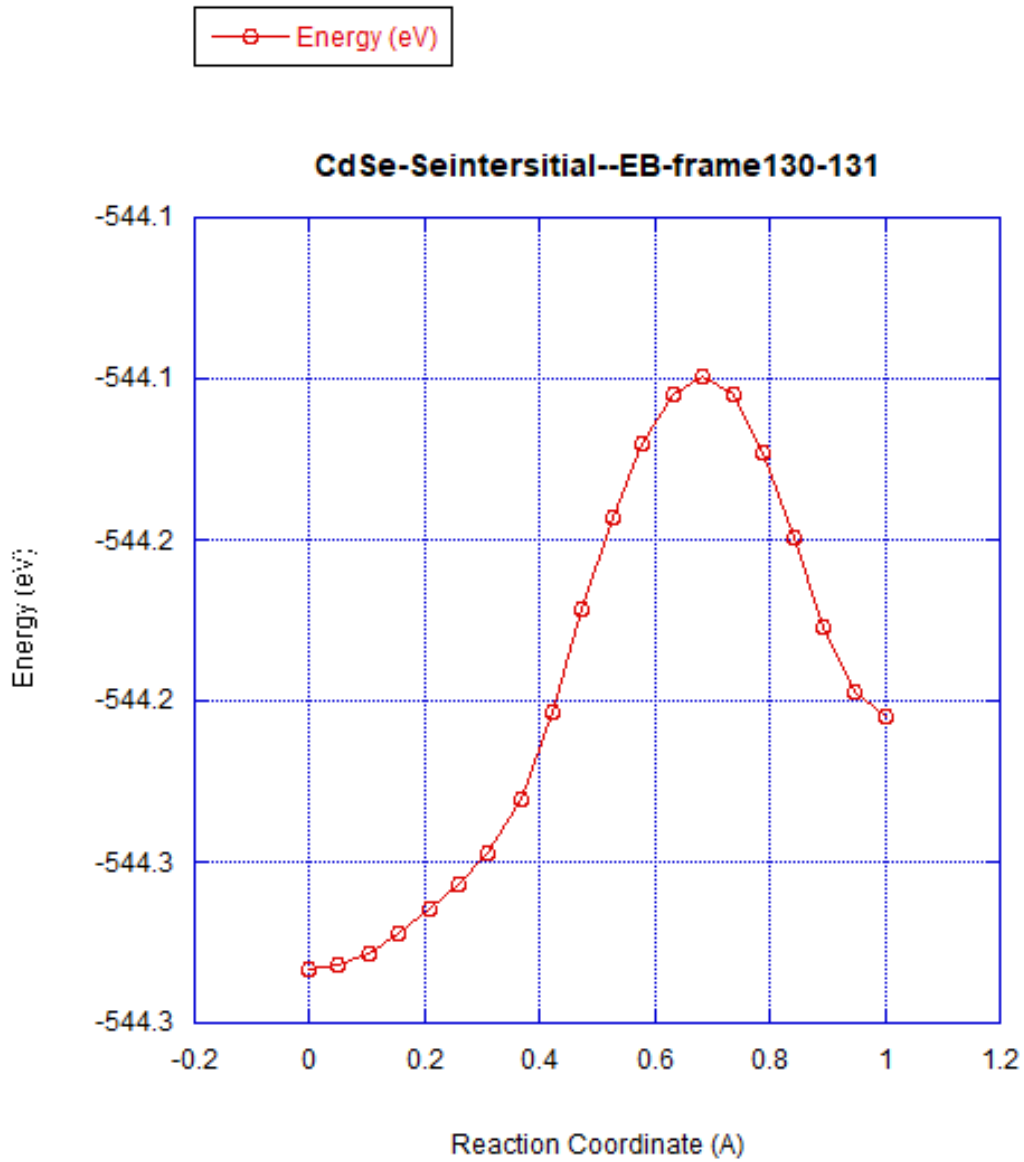


Red = Cd, yellow = Se



White = interstitial, blue = regular crystal structure

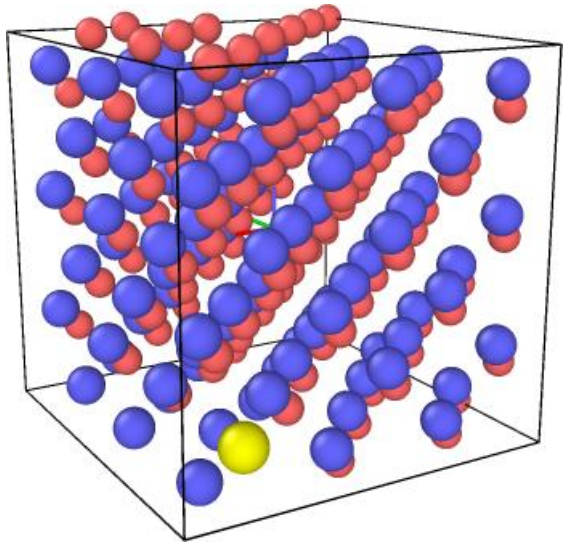
Energy Barriers of Se in CdSe



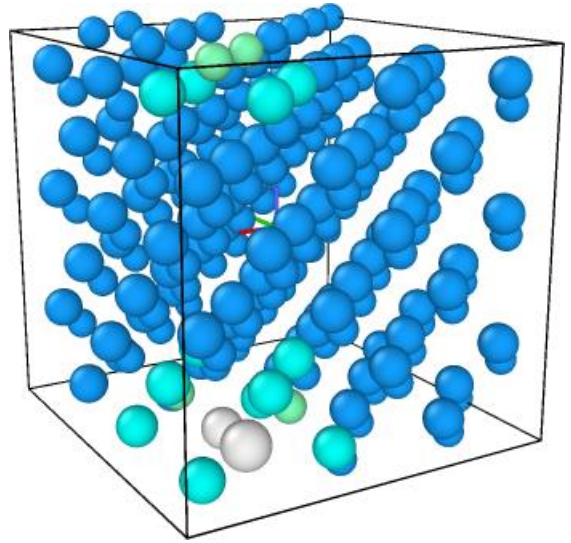
Activation barriers for Se interstitial in Cd**Se:** Table 1

Time	Config No	Particle	Event Typ	Energy LEI	Energy RIC	Barrier 1	Barrier 2	Barrier 3
2.5	5	1	hop	-544.168	-544.016	0.34849		
5.5	11	3	exchange	-544.284	-544.362	0.20725		
8.5	17	3	hop	-544.362	-544.205	0.281		
17.5	35	3	hop	-544.294	-544.284	0.36224		
24	48	3	hop	-544.284	-544.205	0.17008	0.09932	0.24001
32.5	65	169	exchange	-544.294	-544.205	0.17696		
39.5	79	169	hop	-544.205	-544.294	0.31563		
47	94	169	hop	-544.285	-544.017	0.3163	0.06258	0.26731
47.5	95	169	hop	-544.016	-544.168	0.19618		
52	104	3	exchange	-544.294	-544.205	0.17665		
54	108	3	hop	-544.017	-544.168	0.19638		
55	110	3	hop	-544.168	-544.286	0.34541		
56	112	3	hop	-544.284	-544.294	0.34542		
65.5	131	43	exchange	-544.283	-544.205	0.18435		
66	132	43	hop	-544.205	-544.362	0.12357		

Se interstitial in CdTe: initial configuration

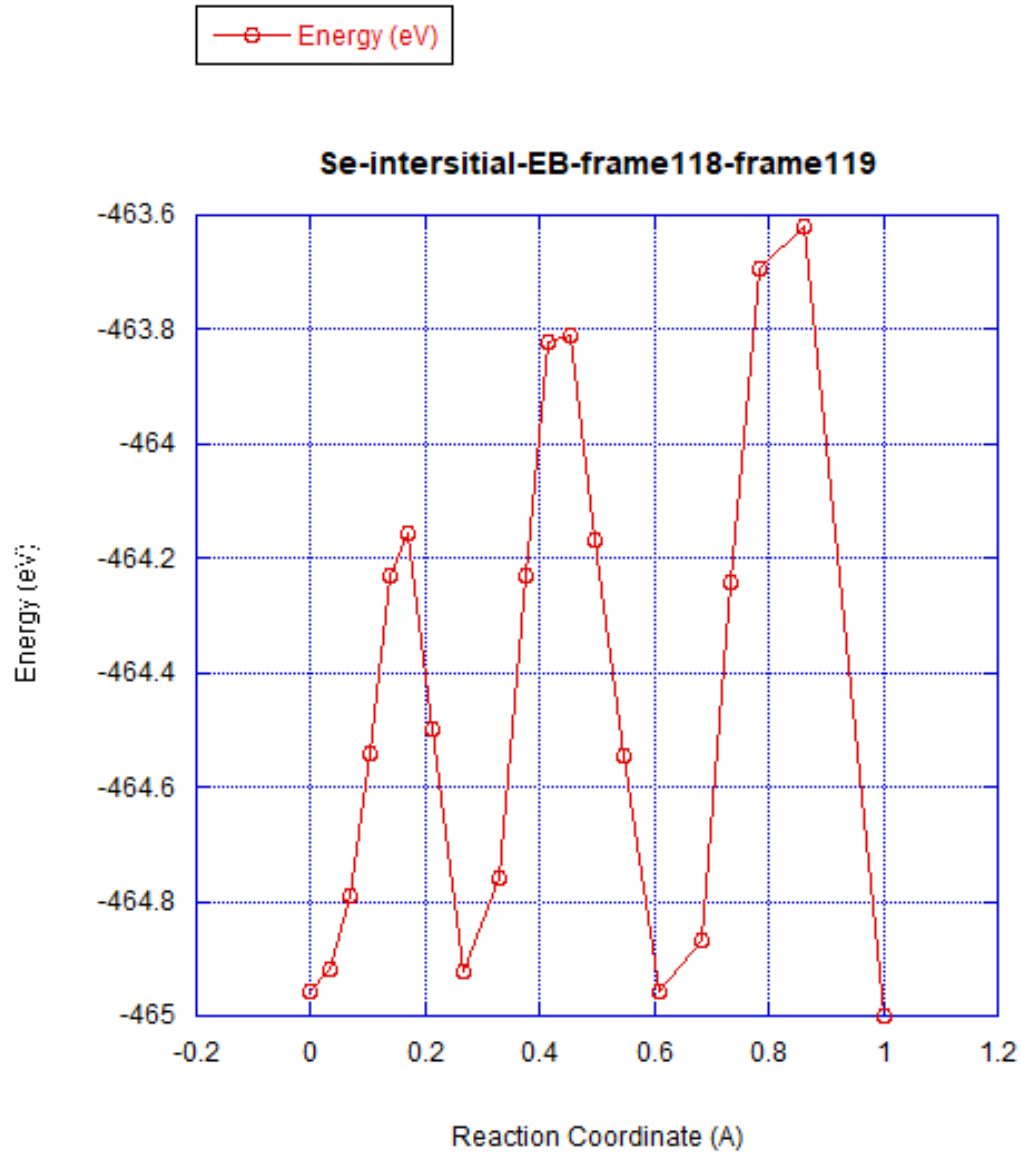


Red = Cd, blue = Te, yellow = Se



White = interstitial, blue = regular crystal structure

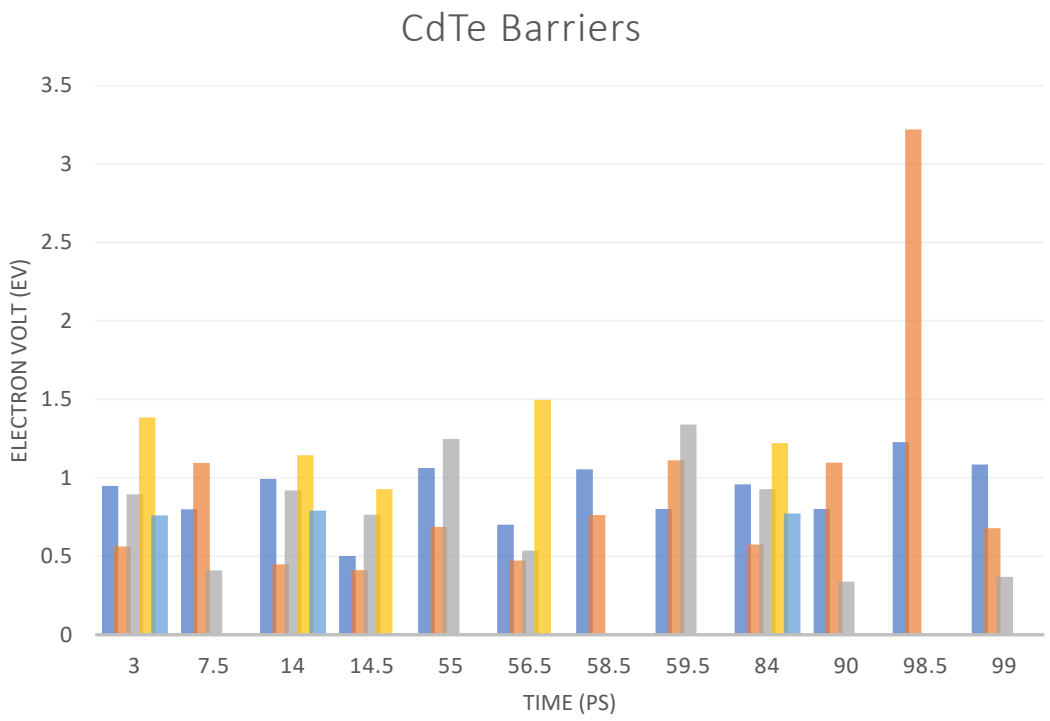
Energy Barriers of Se in CdTe

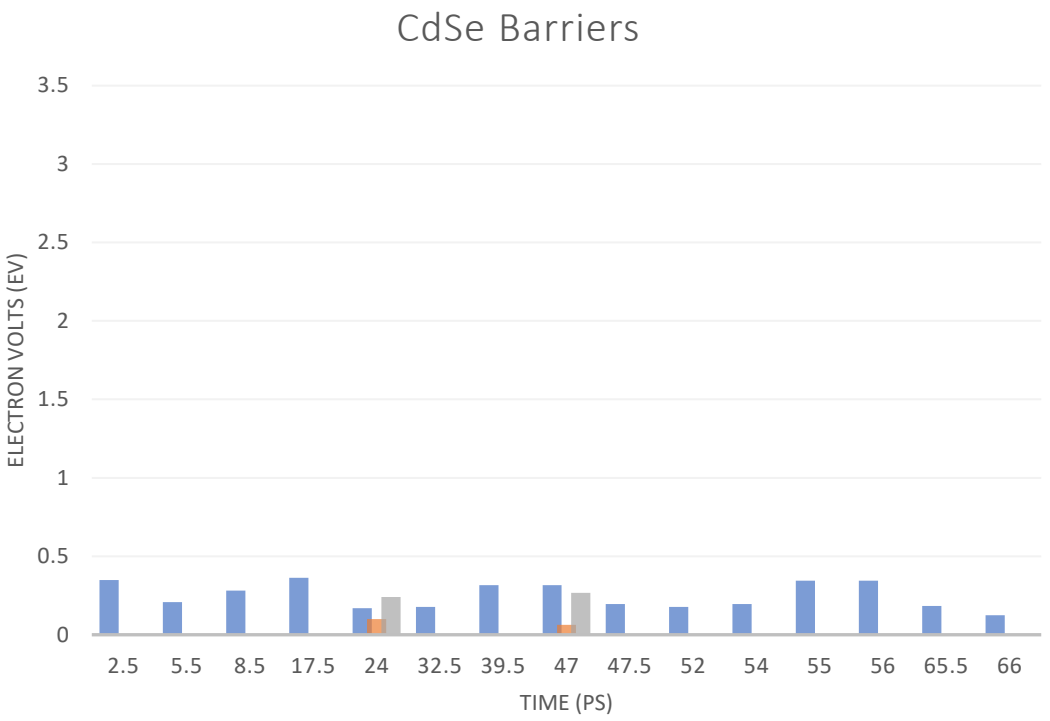


Activation barriers for Se interstitial in Cd**Te**: Table 2

Time	Config No	Particle	Event Typ	Magnitud	Barrier 1	Barrier 2	Barrier 3	Barrier 4	Barrier 5
3	6	1	hop	1.24865	0.94712	0.56326	0.89421	1.38496	0.76071
7.5	15	1	hop	1.25745	0.79923	1.09473	0.40883		
14	28	1	hop	1.26771	0.99352	0.44747	0.91912	1.14406	0.79079
14.5	29	1	hop	1.27098	0.50039	0.41081	0.76436	0.92679	
55	110	1	hop	1.67996	1.06285	0.68733	1.2466		
56.5	113	1	hop	1.66367	0.70014	0.47185	0.53513	1.49605	
58.5	117	1	hop	1.67208	1.05362	0.7614			
59.5	119	1	hop	1.67039	0.80081	1.11151	1.3399		
84	168	1	hop	1.27217	0.95896	0.5754	0.92716	1.2204	0.77221
90	180	1	hop	1.24585	0.80009	1.09702	0.33803		
98.5	197	1	hop	1.23335	1.22798	3.21915			
99	198	1	hop	1.2276	1.08434	0.67843	0.36852		

Comparison of Se in CdTe and Se in CdSe energy barriers.





Conclusions

* Our results indicate that the energy barriers for a Se interstitial to diffuse in CdTe are much larger than the energy barriers needed for a Se interstitial to diffuse in CdSe.

* Further work will be needed to complete these results as well as to study diffusion on longer length-scales.

* Further work will also be needed to determine the overall activation barriers and prefactors for diffusion in each case.