Displacement per Atom Ab Initio Molecular Dynamics Driven Process Design of Crystallographic Novel Fusion Compounds

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Motivation

Fusion reactors are promising **self-sustainable energy generation devices** consisting of a plasma reaction of high energy ionized particles at high temperatures. Current limitations in fusion reactors include those due to the knockoff of highly energized subatomic particles from the ion source into wall linings.

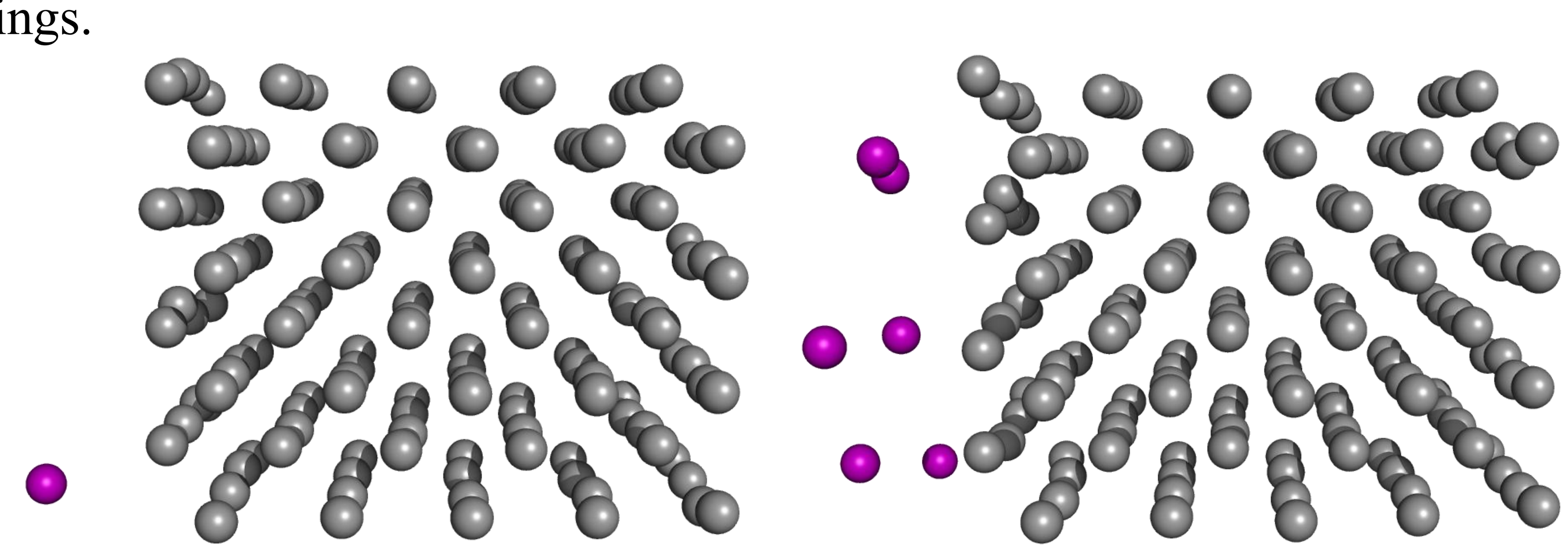

Figure 1: θ = 6.25% (left) and θ = 37.50% (right) cesium covered molybdenum

Background

High-energy particle collisions with wall linings defects. The defects can be characterized by the displacement of the atoms which are dependent on the collision energy, orientation, and the symmetry of the material. The permanent defect formation is correlated with the **threshold displacement energy (E_d).**

Methodology

Second Ion Experiment for Sputtering and TDS Analysis (SIESTA) is the density functional theory software used in this study.

1. Pseudopotential and geometry relaxation
2. Optimized lattice geometry
3. Equilibrated structure at desired temperature
4. Add energy to chosen surface atom

Goal: Model E_d of orientation varied collisions of surface atoms on coverage varying cesium molybdenum systems.

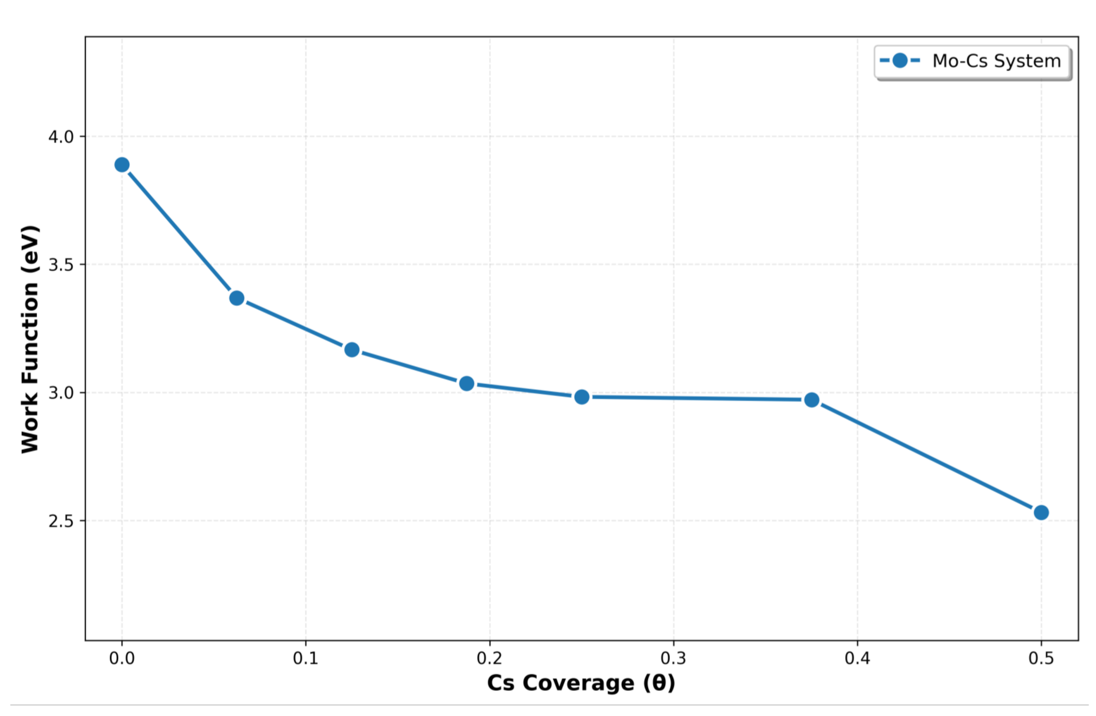

Figure 2: Work function vs cesium coverage

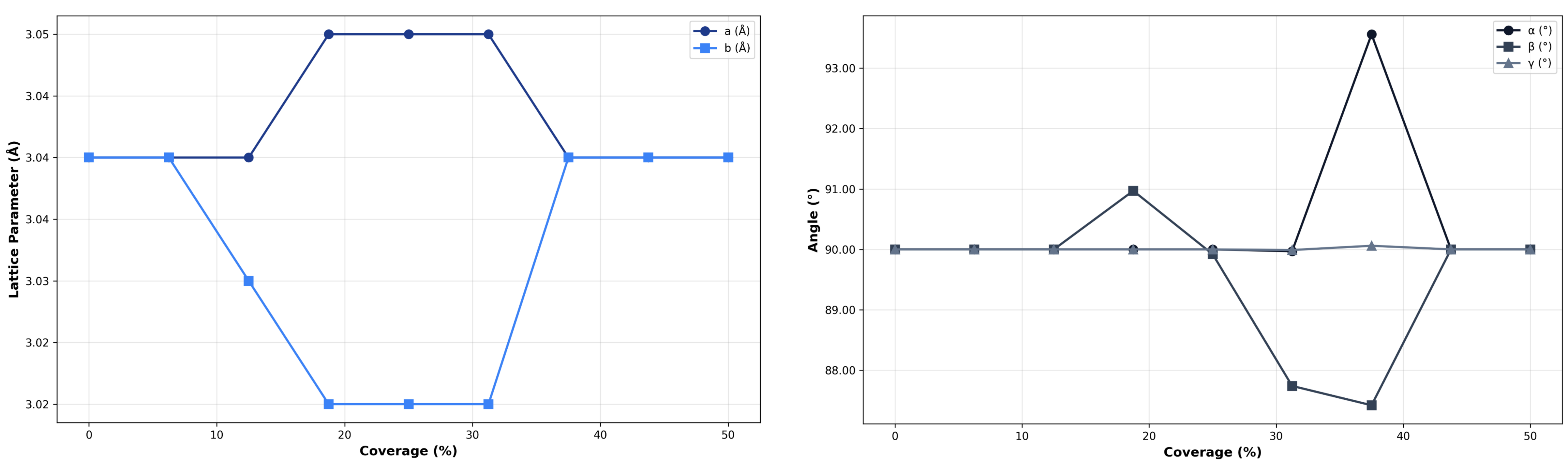

Figure 3: Lattice spacing(left) and angles(right) of varied coverage cesium on molybdenum

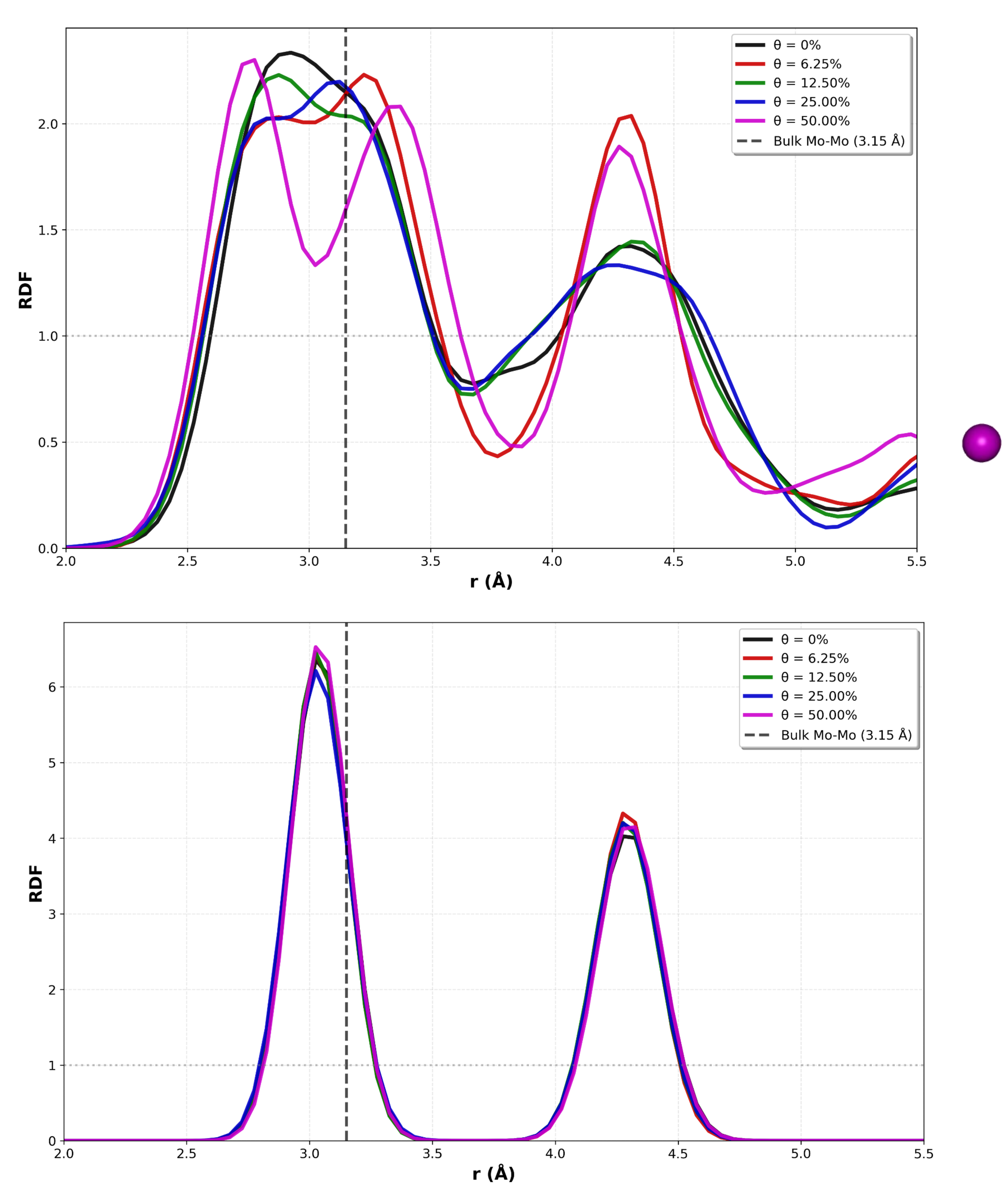

Figure 4: Radial function distribution of top(top) and second(bottom) molybdenum layer

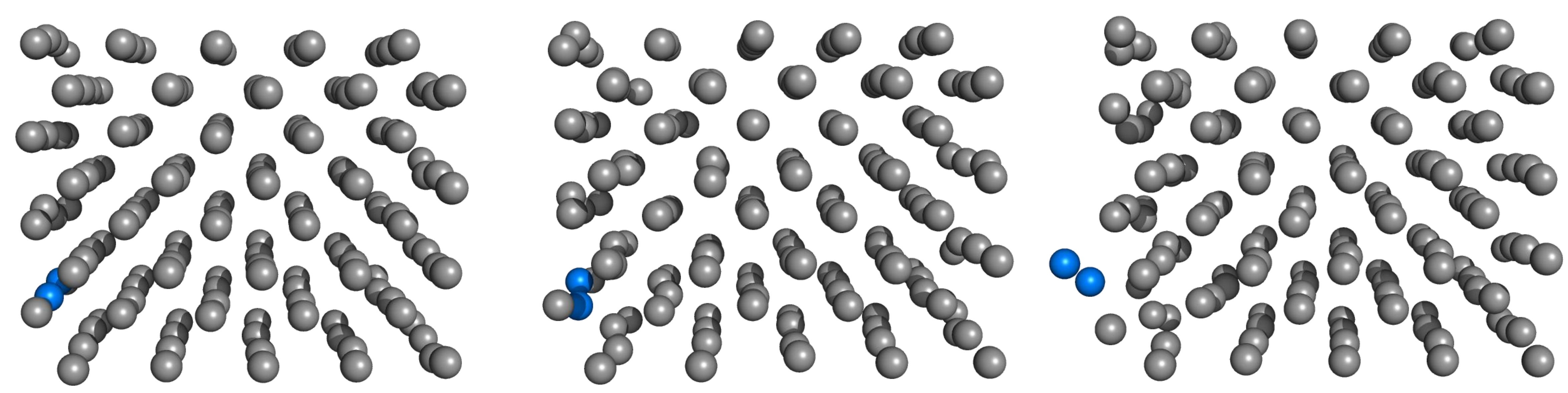

Figure 5: θ = 6.25% at equilibrium(left), and after 45 eV(middle) and 50 eV(right) 211 collision

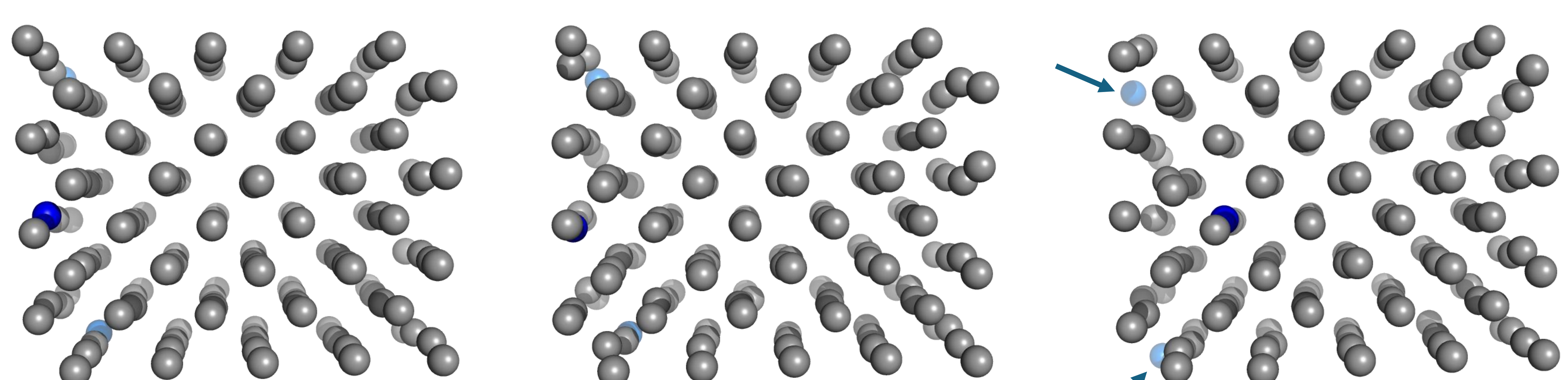

Figure 6: θ = 0% at equilibrium(left), and after 25 eV(middle) and 26 eV(right) 100 collision

Direction	0%	6.25%	12.50%	18.75%	50.0%
[100]	26	25-30	20-40	20-40	20-40
[111]	26	20-25	20-40	15-20	<20
[211]	40-60	45-50	40-60	15-20	<20

Table 1: E_d values for various cesium coverages on a molybdenum slab

Future Works

Future work will include doping the Mo slab with defects with varied concentrations and varying the face of Mo on which the Cs is deposited, as this alters the work function of the materials. Future works include using other low-work function materials to optimize the wall lining material.

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Citations

1. Said, Halima, et al. "Ab Initio Molecular Dynamics Investigation of Cs Adsorption on Mo(0 0 1): Beyond a Single Monolayer Coverage." Applied Surface Science, vol. 559, Sept. 2021, p. 149822, https://doi.org/10.1016/j.apsusc.2021.149822.
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