NOMATEN
Centre of Excellence in Multifunctional Materials for Industrial and Medical Applications

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Threshold Displacement Energy Study in Tungsten: Combining Machine Learning and Classical MD Simulations

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SCAN ME

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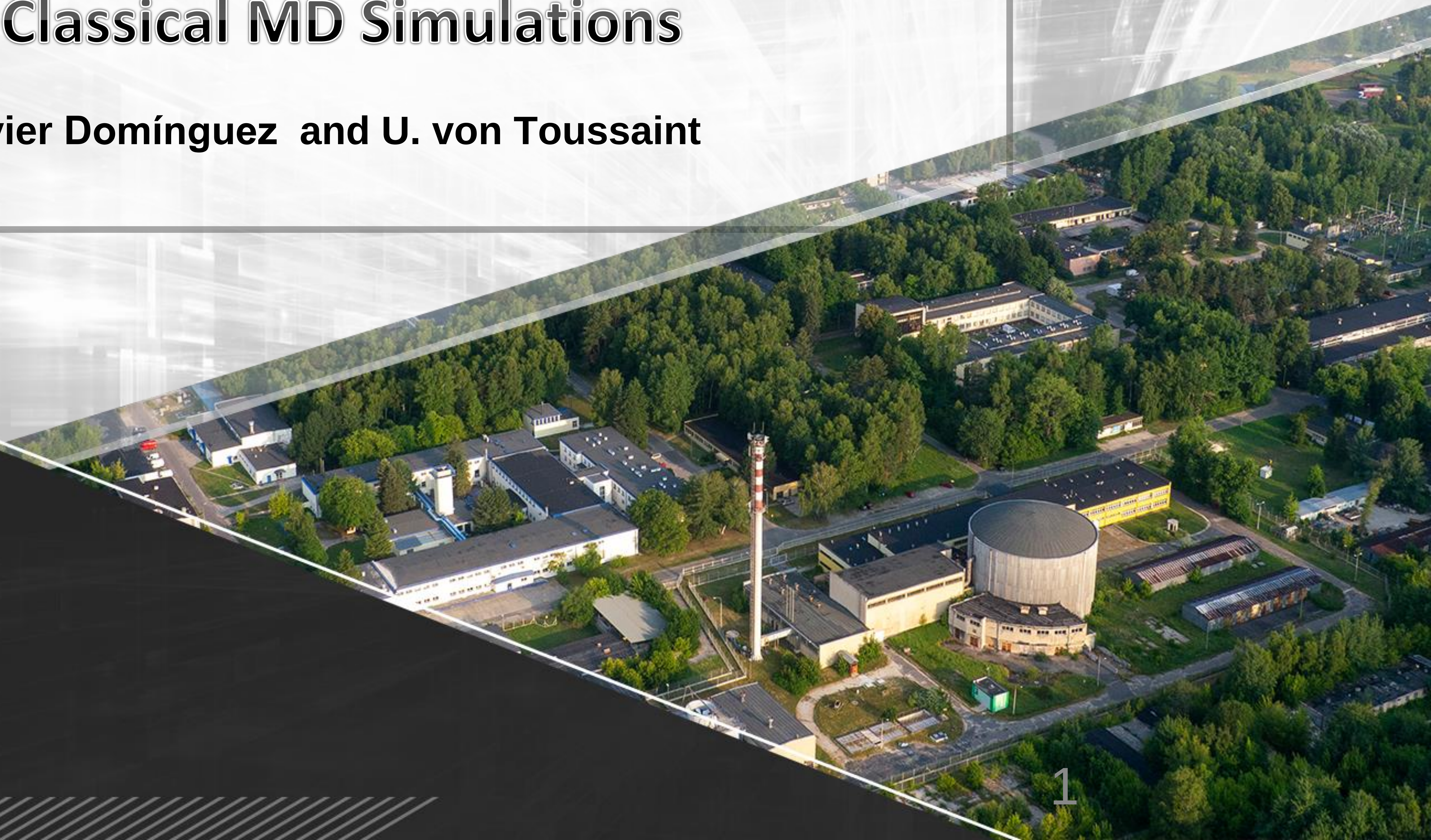
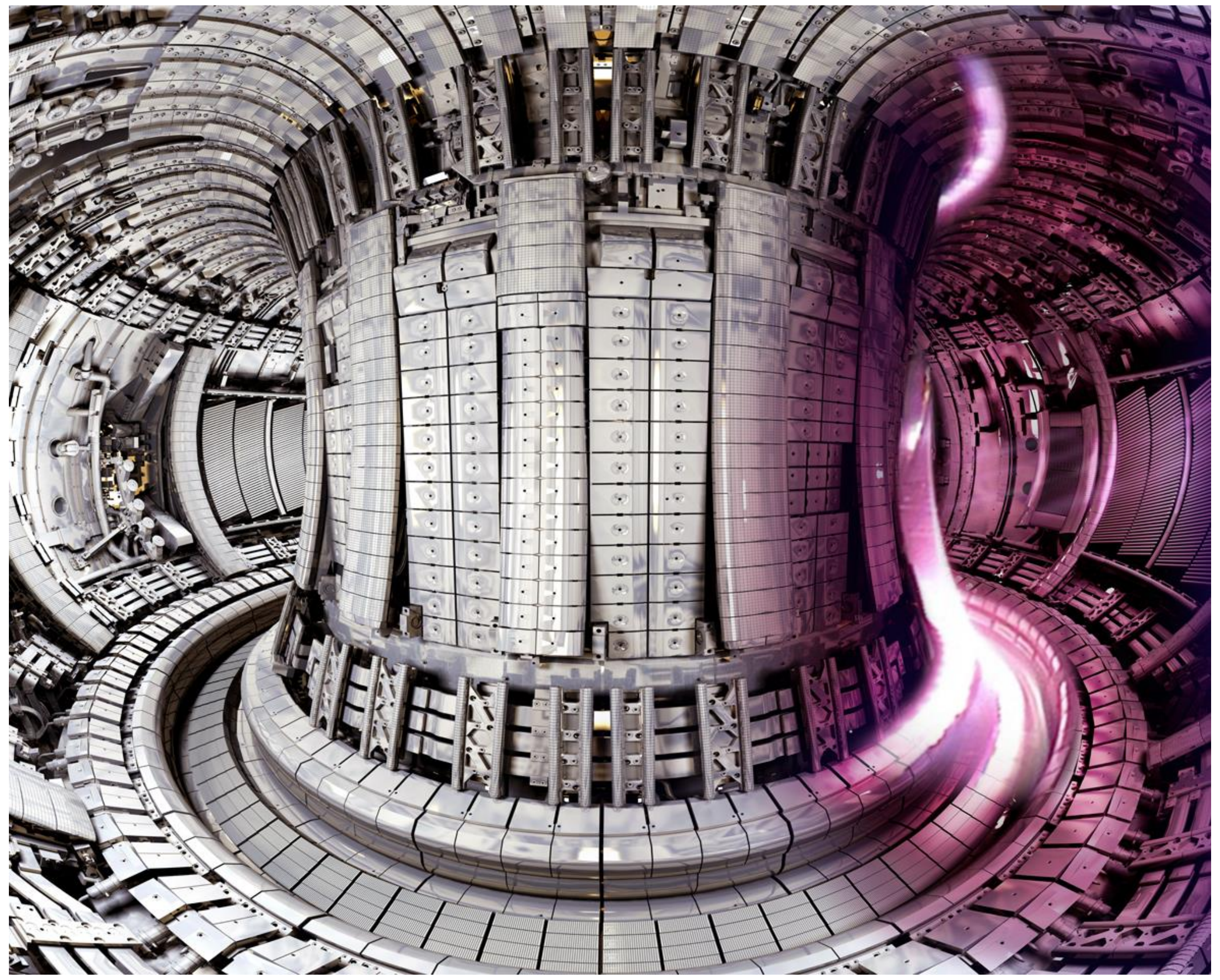


Motivation: Optimal materials for extreme operating conditions

Promising mechanical properties: high yield strength, high thermal stability and hardness, high-temperature strength, good wear and fatigue resistance, and excellent corrosion resistance

- Refractory BCC mixed materials for designing next generation of fusion reactors.



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Computational methods

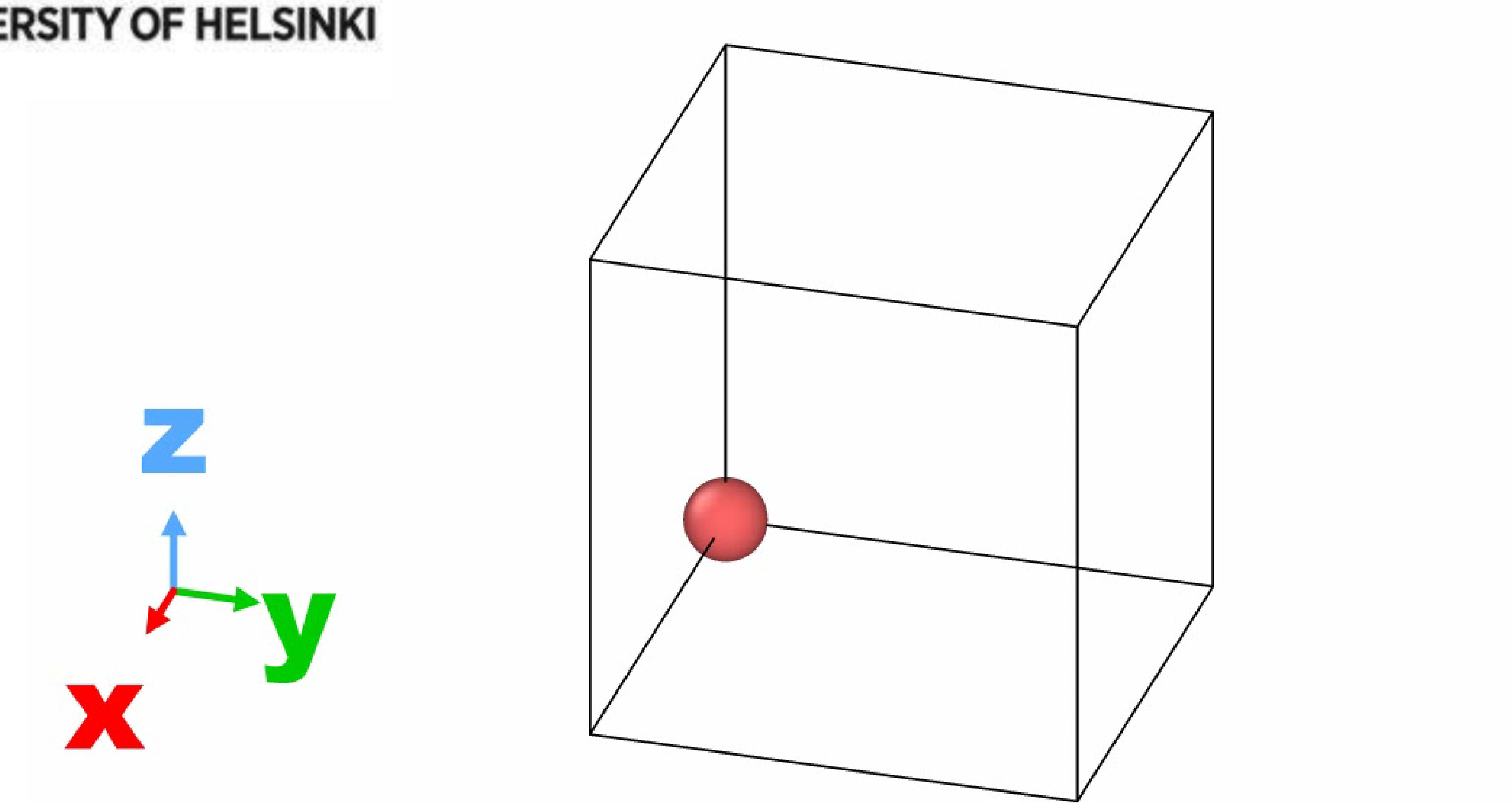
- MD simulations for collision cascades
- A simulation cell of 4 nm^3 size
- 20 velocities per PKA with random velocities orientations
- PKA range from 20 to 100 eV
- 10 ps simulation time
- IP: TabGAP; ABOP (Tersoff); EAM.
- W samples with 0.05 and 1.0 at %D

MLIP for W

In collaboration with:
University of Helsinki
1. **J. Byggmastar**
2. F. Djurabekova
3. K. Nordlund

UNIVERSITY OF HELSINKI

DFT calculations



Gaussian Approximation Potential Framework:

$$E_{\mathrm{tot}} = \sum_{i<j}^{N} V_{\mathrm{pair}}(r_{ij}) + \sum_{i}^{N_{\mathrm{d}}} E^{i}_{\mathrm{GAP}},$$

$$E^{i}_{\mathrm{GAP}} = \delta^{2}_{2\mathrm{b}} \sum_{j}^{M_{2\mathrm{b}}} \alpha_{j,2\mathrm{b}} K_{2\mathrm{b}}(\vec{q}_{i,2\mathrm{b}}, \vec{q}_{j,2\mathrm{b}}) + \delta^{2}_{\mathrm{mb}} \sum_{j}^{M_{\mathrm{mb}}} \alpha_{j,\mathrm{mb}} K_{\mathrm{mb}}(\vec{q}_{i,\mathrm{mb}}, \vec{q}_{j,\mathrm{mb}}),$$

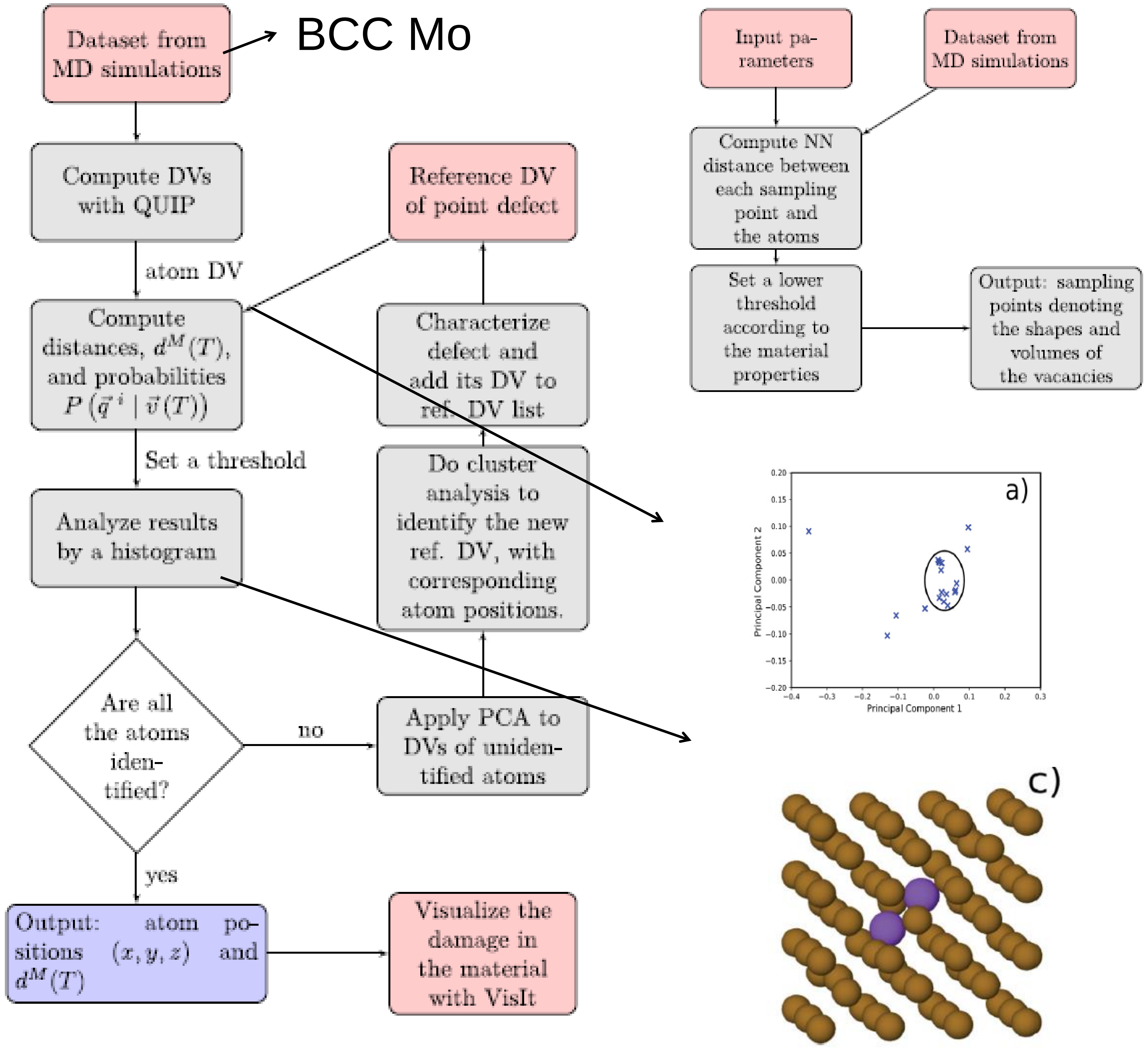
Table 2. Physical properties of molybdenum (cohesion energy, $E_{\mathrm{coh.}}$; melting temperature, $T_{\mathrm{melt.}}$; SIA and vacancy formation energies, E_{f}; and vacancy migration energy, $E^{\mathrm{vac.}}_{\mathrm{mig.}}$) obtained by GAP [15] and EAM [10], as reported in the literature [15], and their comparison to experimental measurements [25].

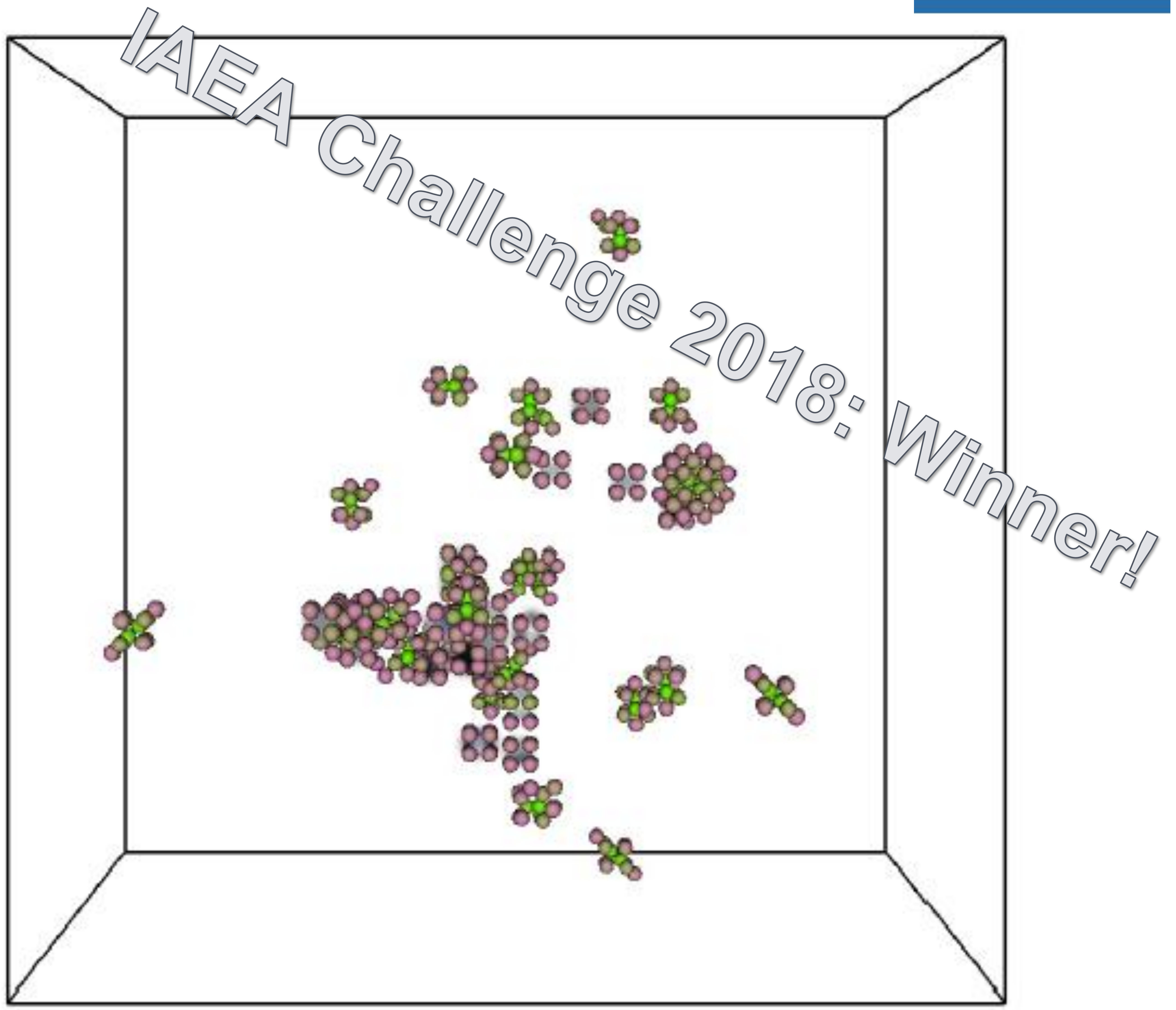
	EAM	GAP	Expt.
$E_{\mathrm{coh.}}$ (eV atom^{-1})	−6.82	−6.288	−6.821
$T_{\mathrm{melt.}}$ (K)	3080 ± 20	2750 ± 10	2895
$E_{\mathrm{f}}^{\langle 111\rangle}$ (eV)	7.19	7.56	—
$E_{\mathrm{f}}^{\langle 110\rangle}$ (eV)	6.95	7.61	—
$E_{\mathrm{f}}^{\langle 100\rangle}$ (eV)	7.18	8.99	—
$E_{\mathrm{f}}^{\mathrm{octa}}$ (eV)	7.56	9.00	—
$E_{\mathrm{f}}^{\mathrm{tetra}}$ (eV)	7.35	8.44	—
$E_{\mathrm{f}}^{\mathrm{vac.}}$ (eV)	2.55	2.84	3.0–3.24
$E_{\mathrm{mig}}^{\mathrm{vac.}}$ (eV)	1.28	1.28	1.35–1.62

Numerical setup:
1. 0.5-10 KeV of PKA
2. 300K sample temperature
3. [001] crystal orientation
4. EAM+ZBL+FS vs GAP

[1] J. Byggmastar, K. Nordlund, and F. Djurabekova. Phys. Rev. Materials 4, 093802 (2020)
[2] F. J. Dominguez, J. Byggmastar, K. Nordlund et al. Modelling Simul. Mater. Sci. Eng. 29, 055001 (2021).
[3] F. J. Dominguez, J. Byggmastar, K Nordlund et al. Nuclear Materials and Energy 22, 100724 (2020)

Fingerprinting and Visualization Analyzer of Defects (FaVAD).



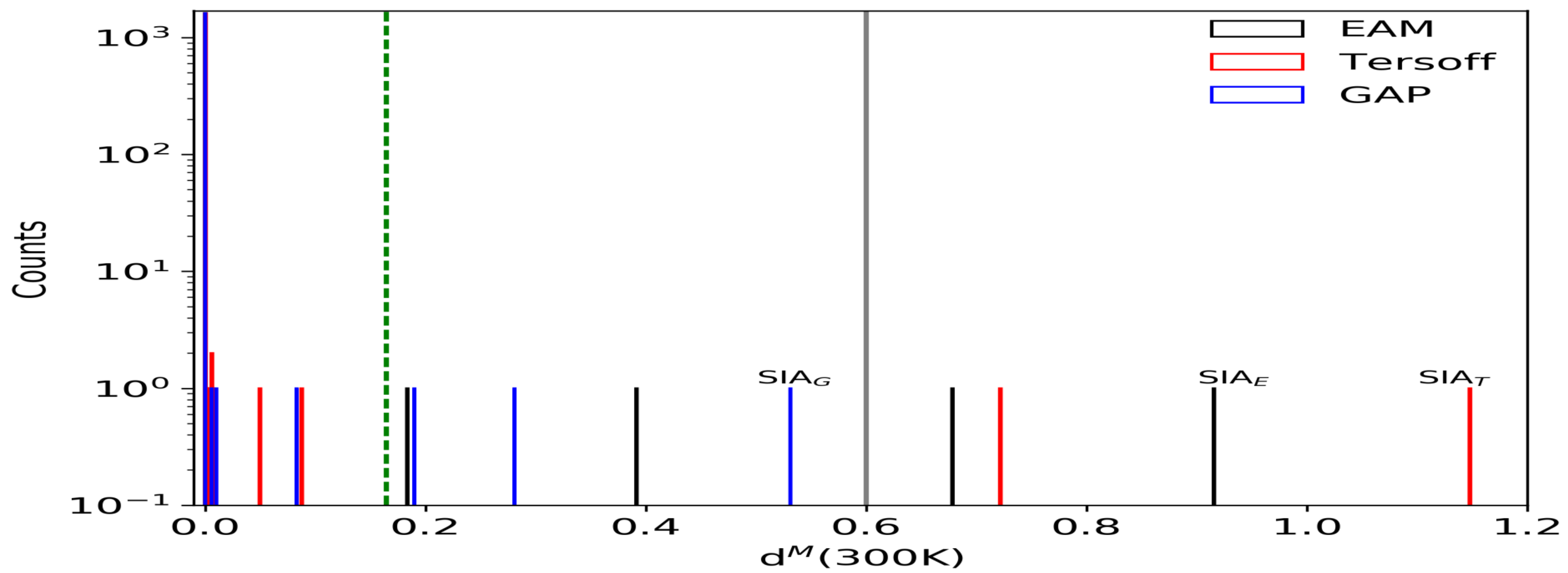


Defect classified for Mo at 50 keV PKA

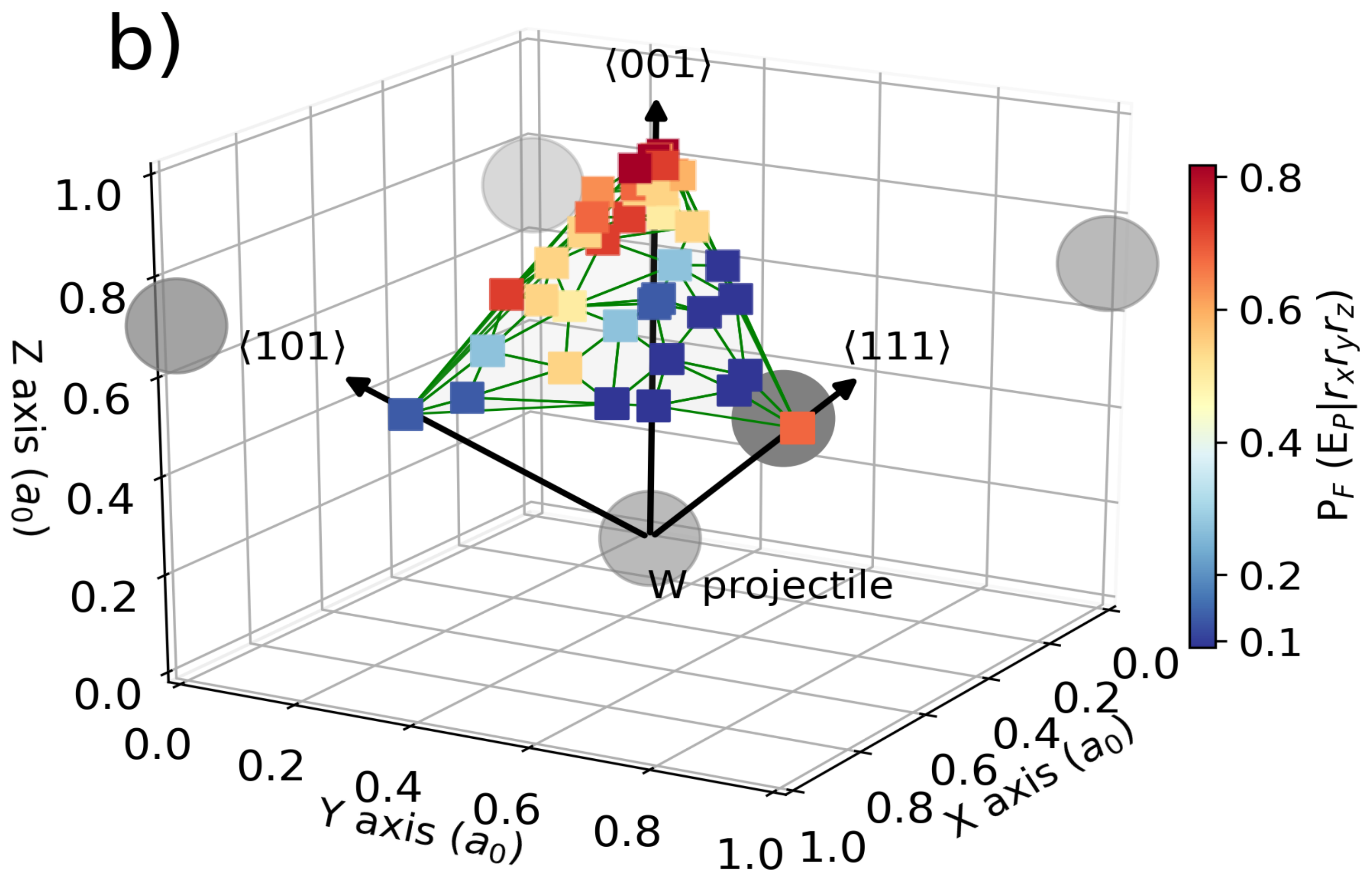
http://libatoms.github.io/QUIP/

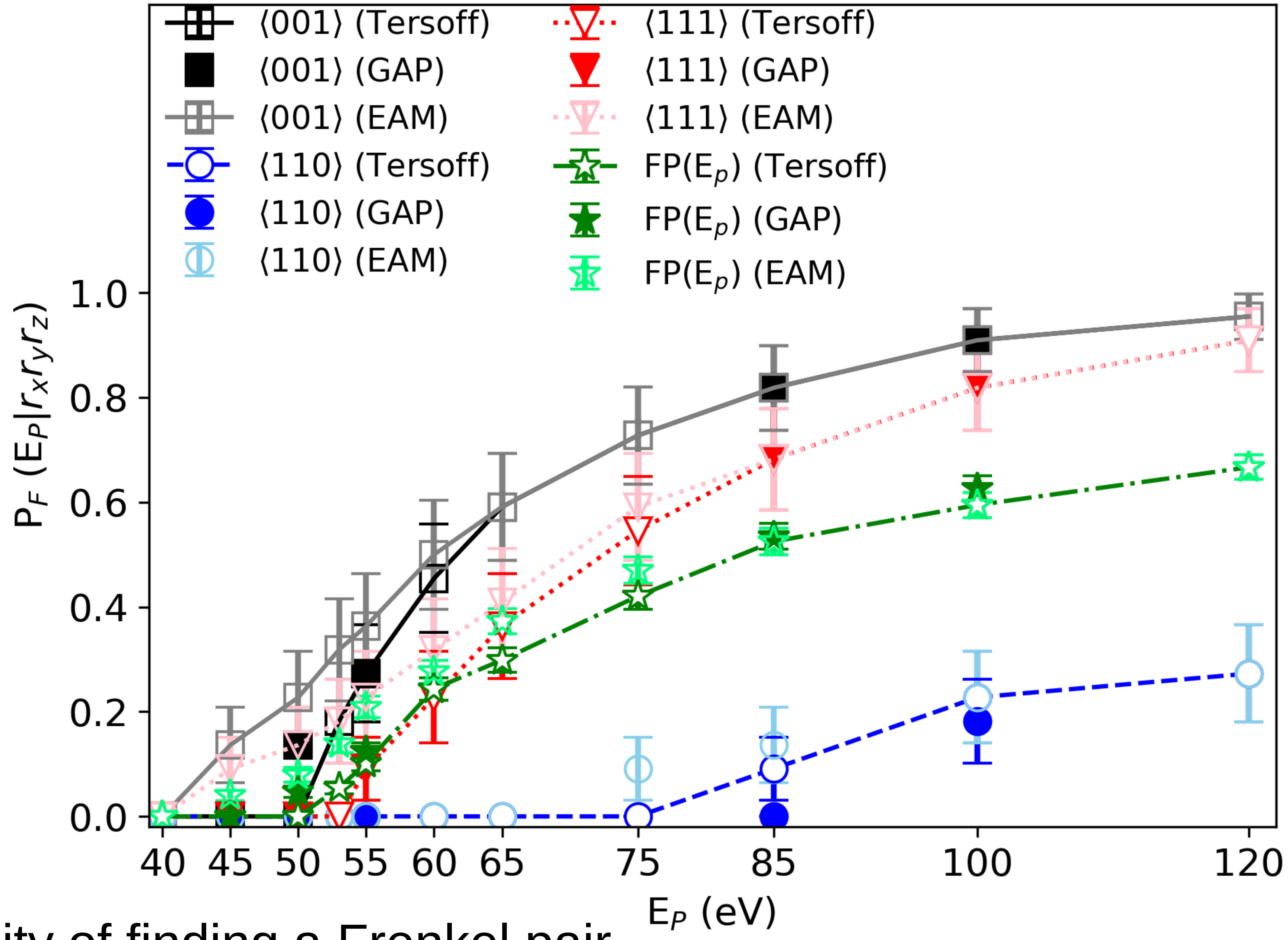
U. Von Toussaint, F. J. Dominguez Gutierrez et al. Comp. Phys. Comm. 262, 107816 (2021)

Results: pure W sample



Identification of defect in W with Favad for a single collision cascade



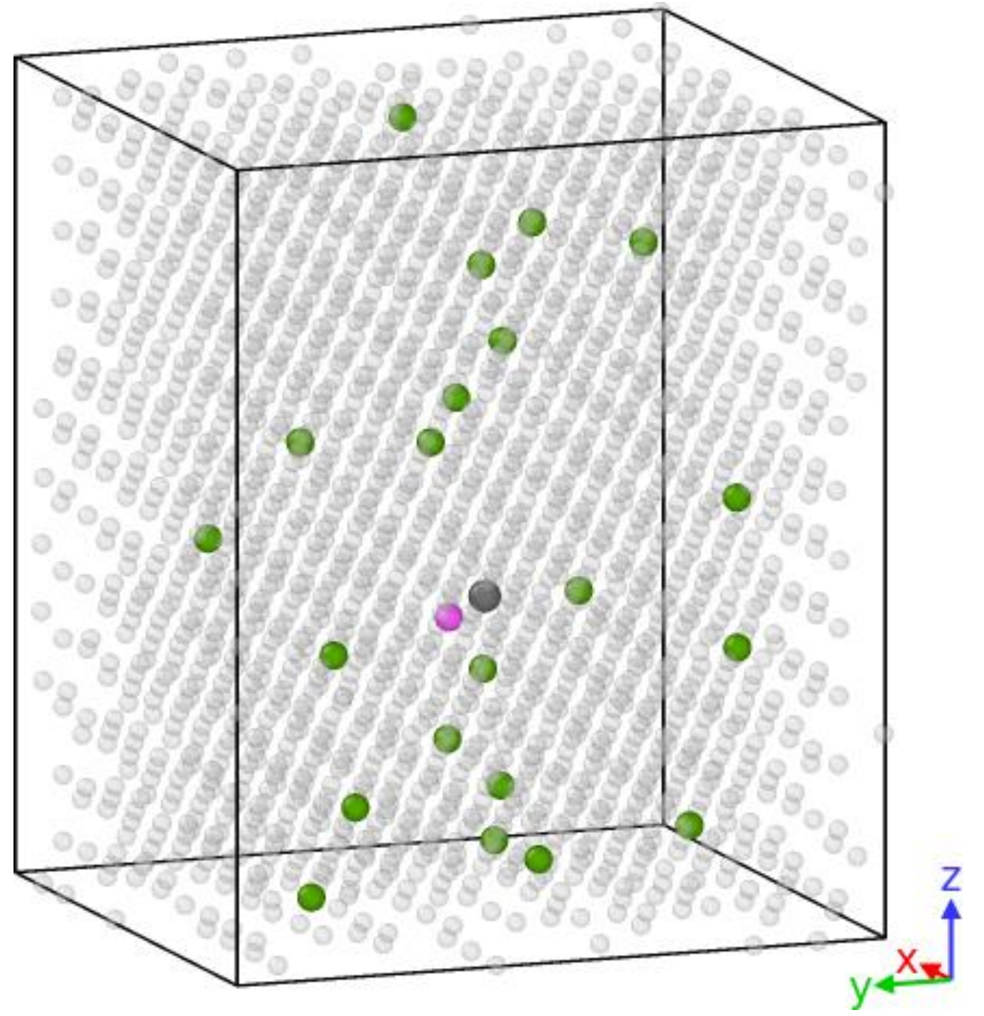


Probability of finding a Frenkel pair formed for a given velocity direction

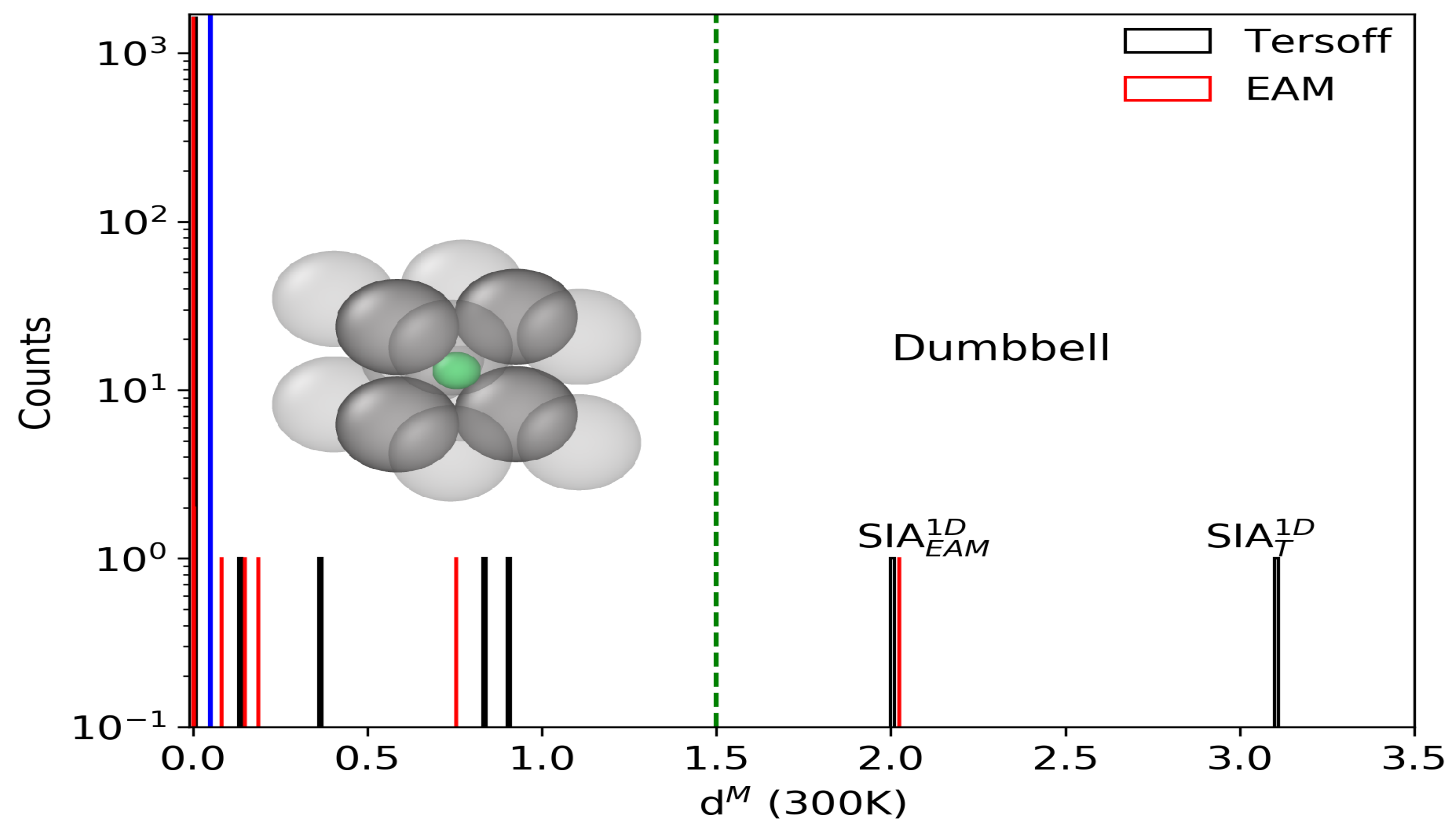
F. J. Dominguez. NIMP-B 512, 38 (2022)

G. Wei et al. J. Nucl. Materials 583, 154534 (2023)

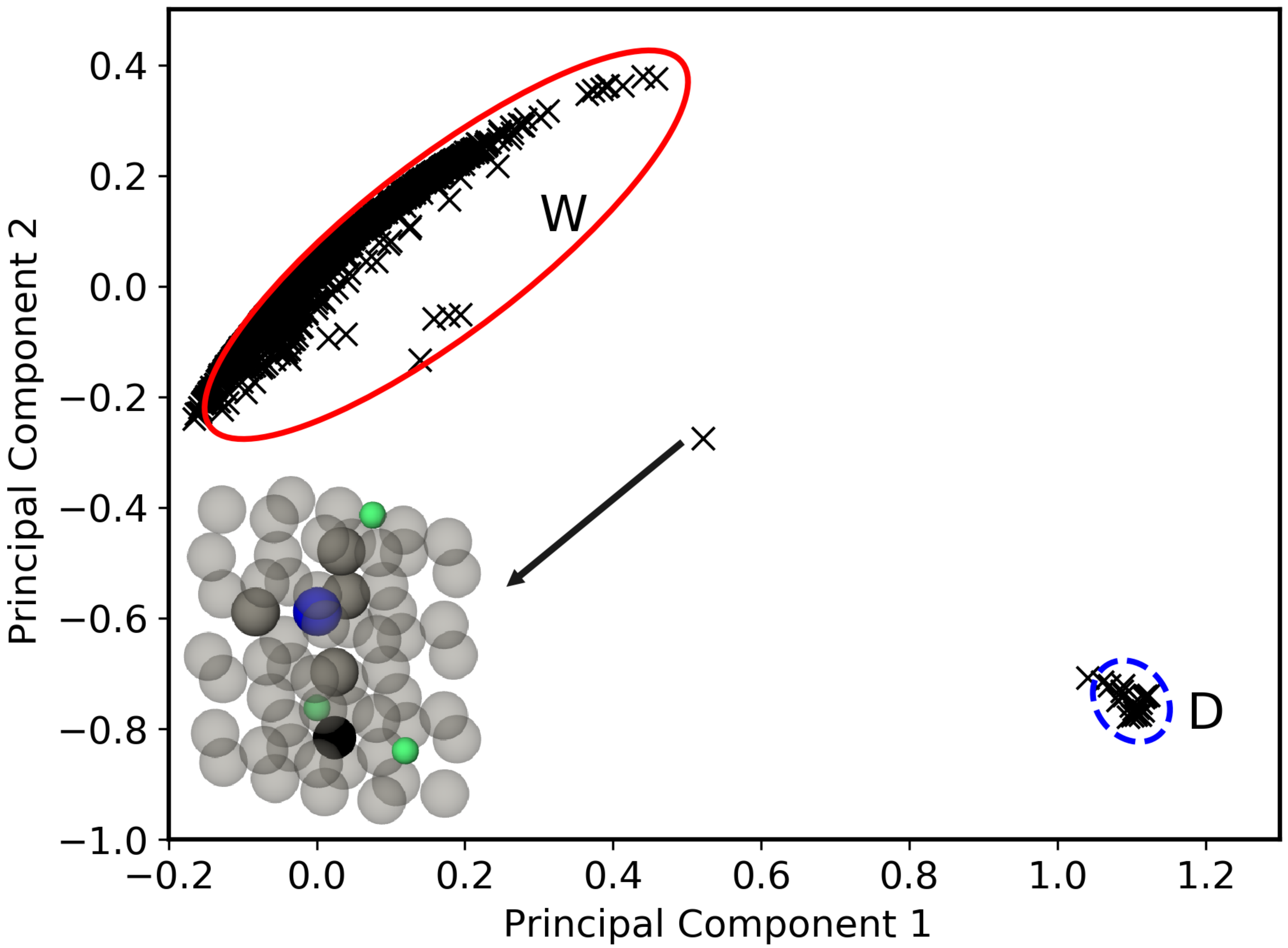
Results: W-D sample



Sample preparation of W-D and D atoms identified with Favad



Identification of defect in W-D with Favad for a single collision cascade (0.05% at D)



Identification of defect in W-D with Favad for a single collision cascade (1.0% at D)

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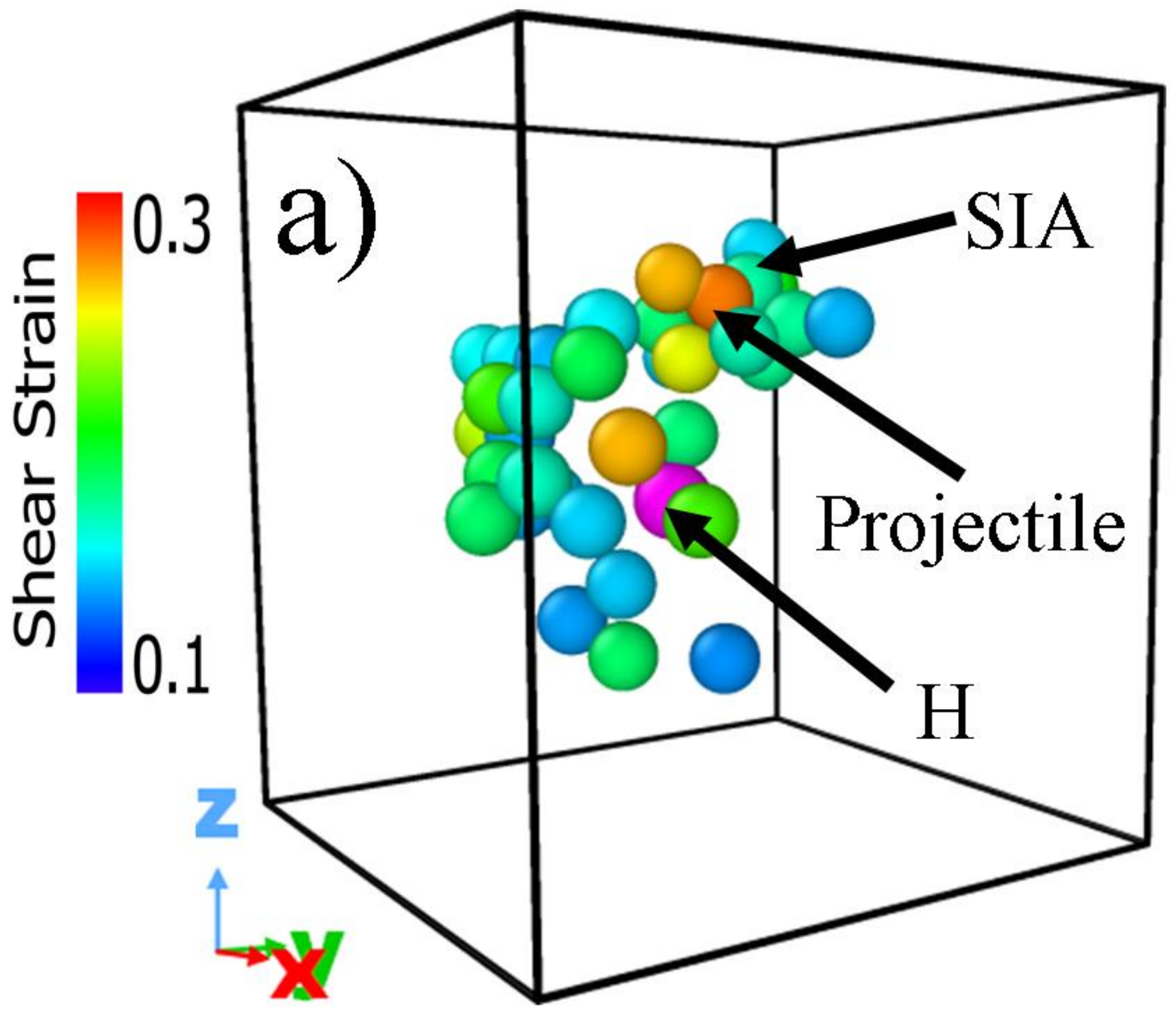
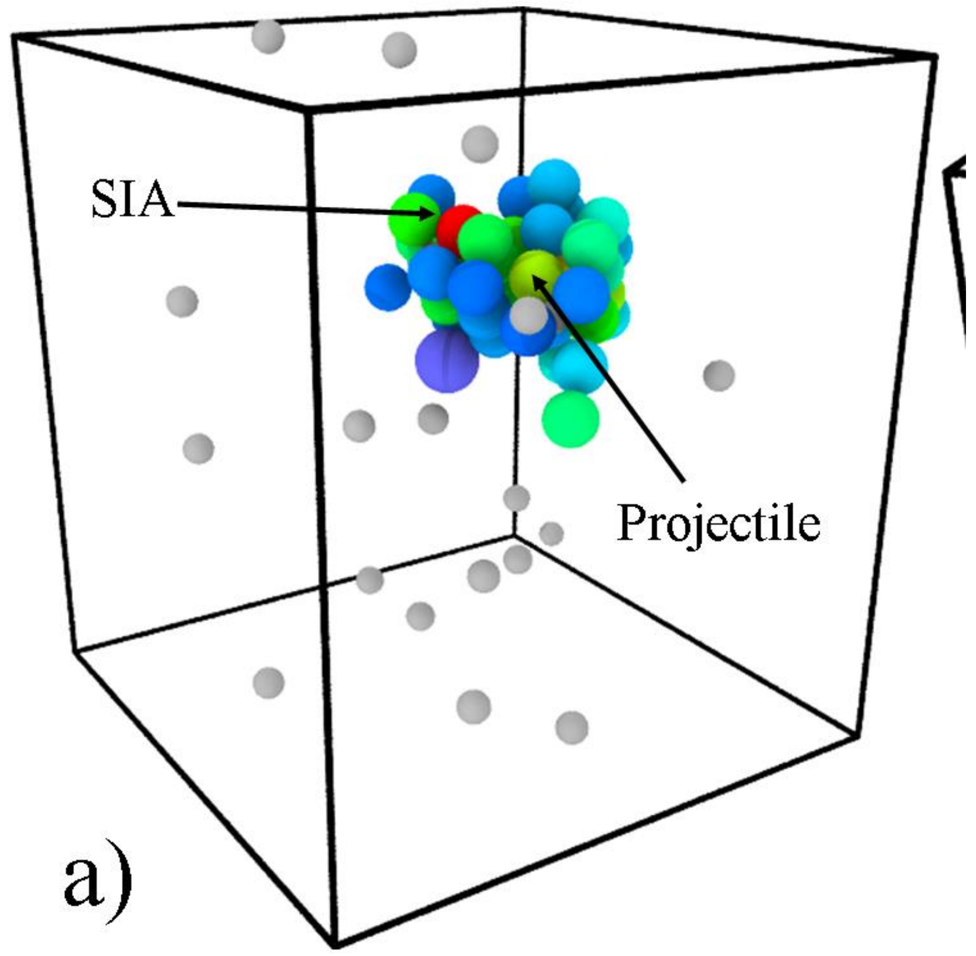
Results: W-D sample

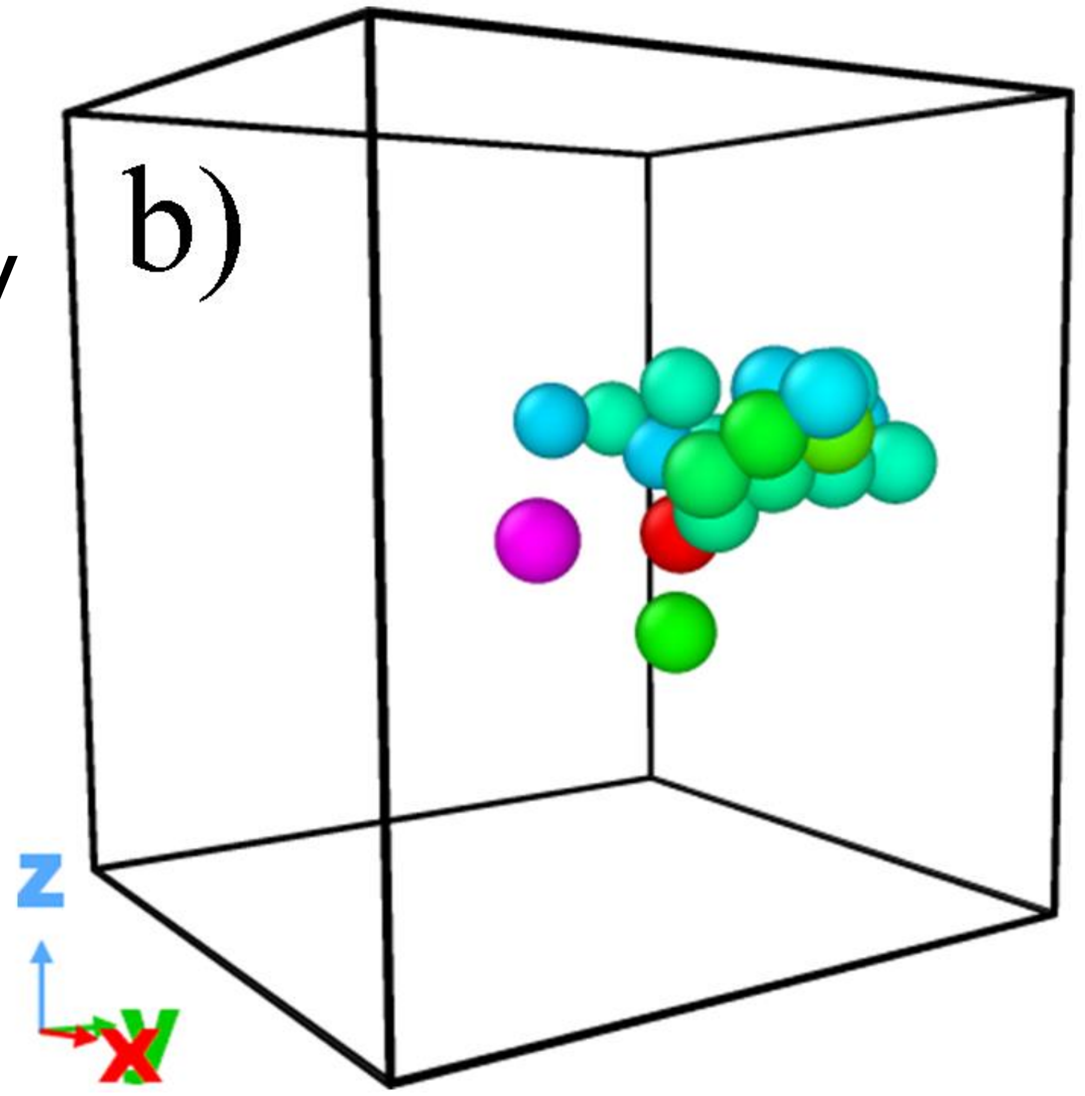


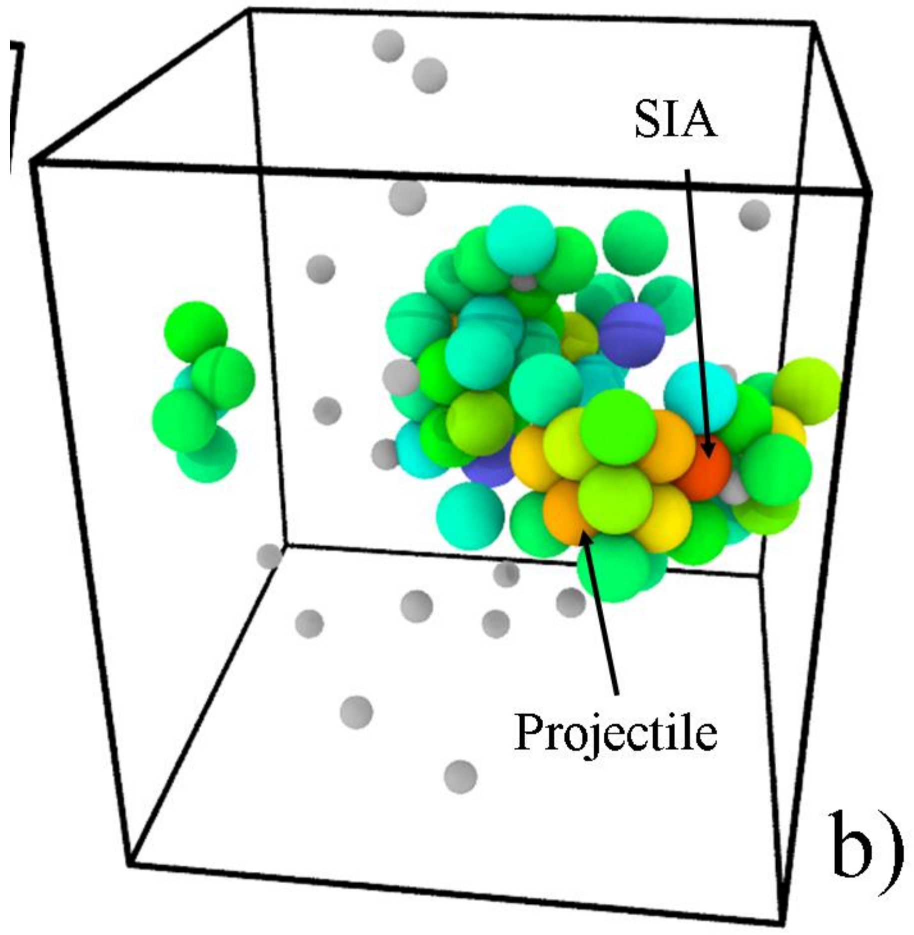
Collision cascade at 75 eV for 0.05% at D; with a projectile close to D



Collision cascade at 75 eV for 1.0% at D; with a projectile close to D

Collision cascade at 75 eV for 0.05% at D; with a projectile far from D



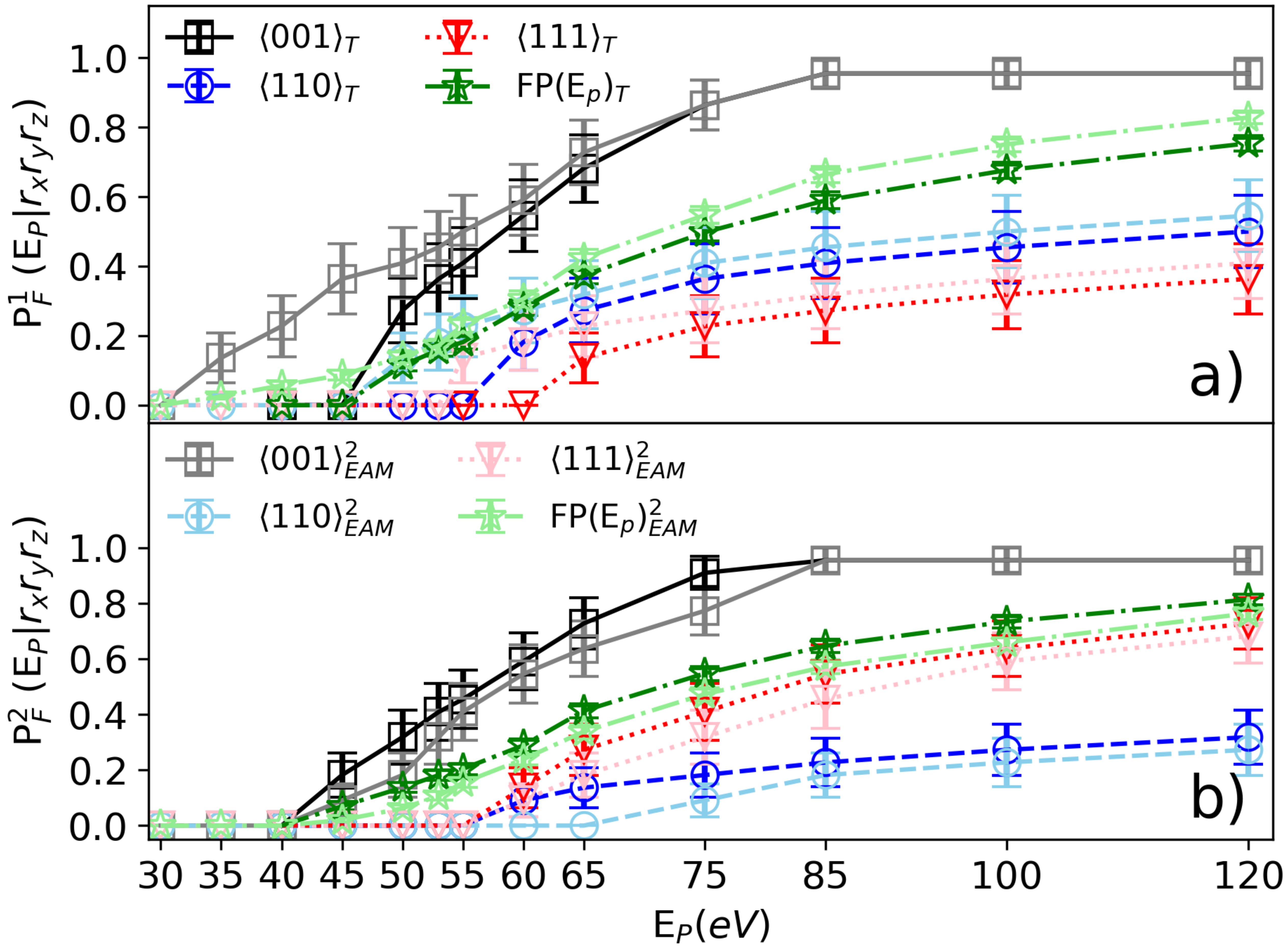


Collision cascade at 75 eV for 1.0% at D; with a projectile far from D

Results: W-D sample with 1.0% at D

Projectile is next to D atoms

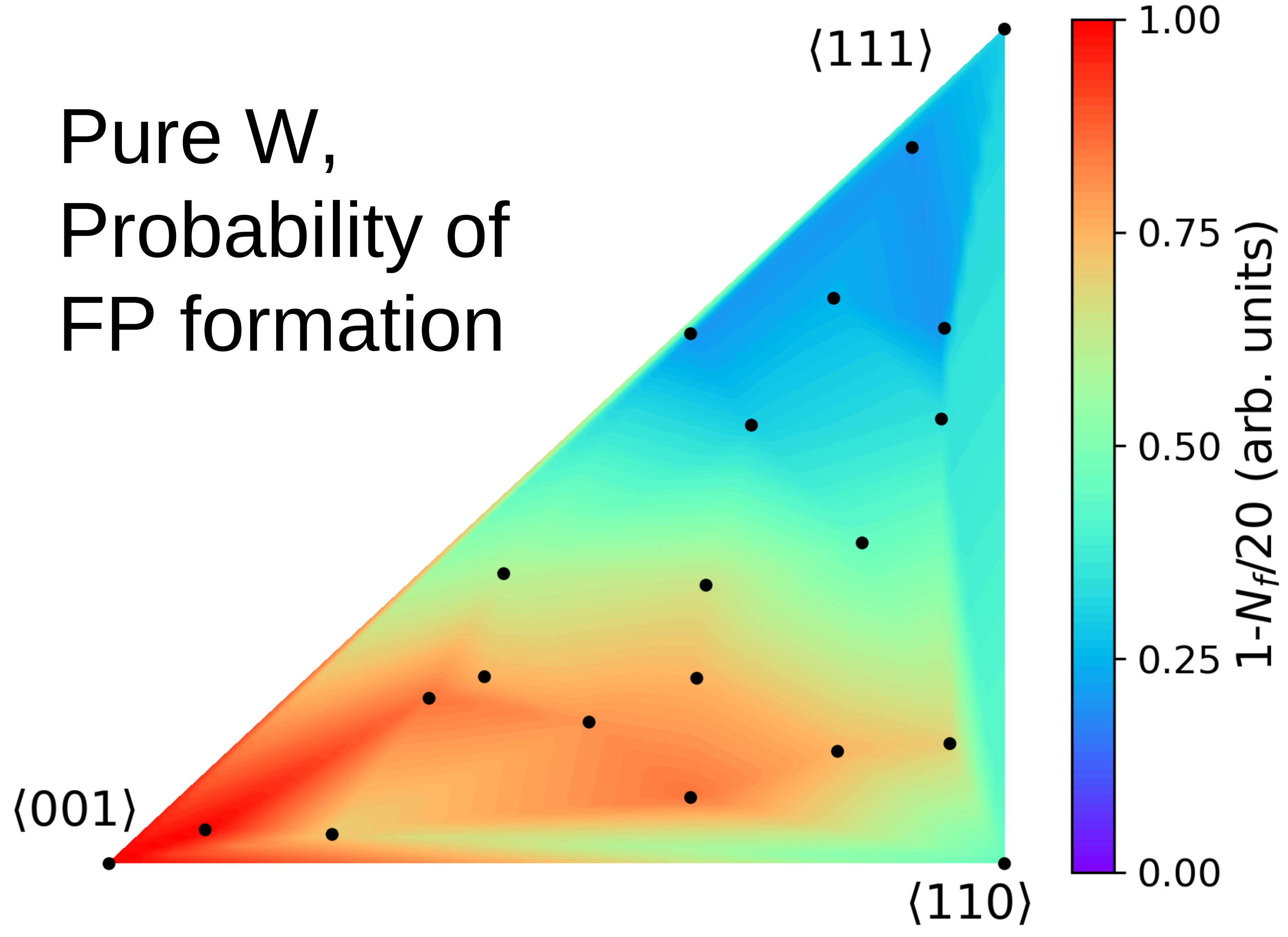
Projectile is far from D atoms



Concluding remarks

From our results for the W samples, the TDE value is 53 eV for Tersoff ZBL, 50 eV for GAP, and 45 eV for EAM on the ⟨001⟩ velocity direction. We notice that a TDE of 85-90 eV is required to create a Frenkel pair in all the velocity orientation of the projectile

Pure W, Probability of FP formation



The TDE is decreased by 5 eV for W-D samples when the projectile is in the vicinity of D atoms

W sample at 35 K			
Method	⟨001⟩	⟨110⟩	⟨111⟩
Tersoff ZBL	47	110	53
GAP	45.5	78	51.5
EAM	42	100	41
Exp.	42 ± 1	70 ± 1	44 ± 1

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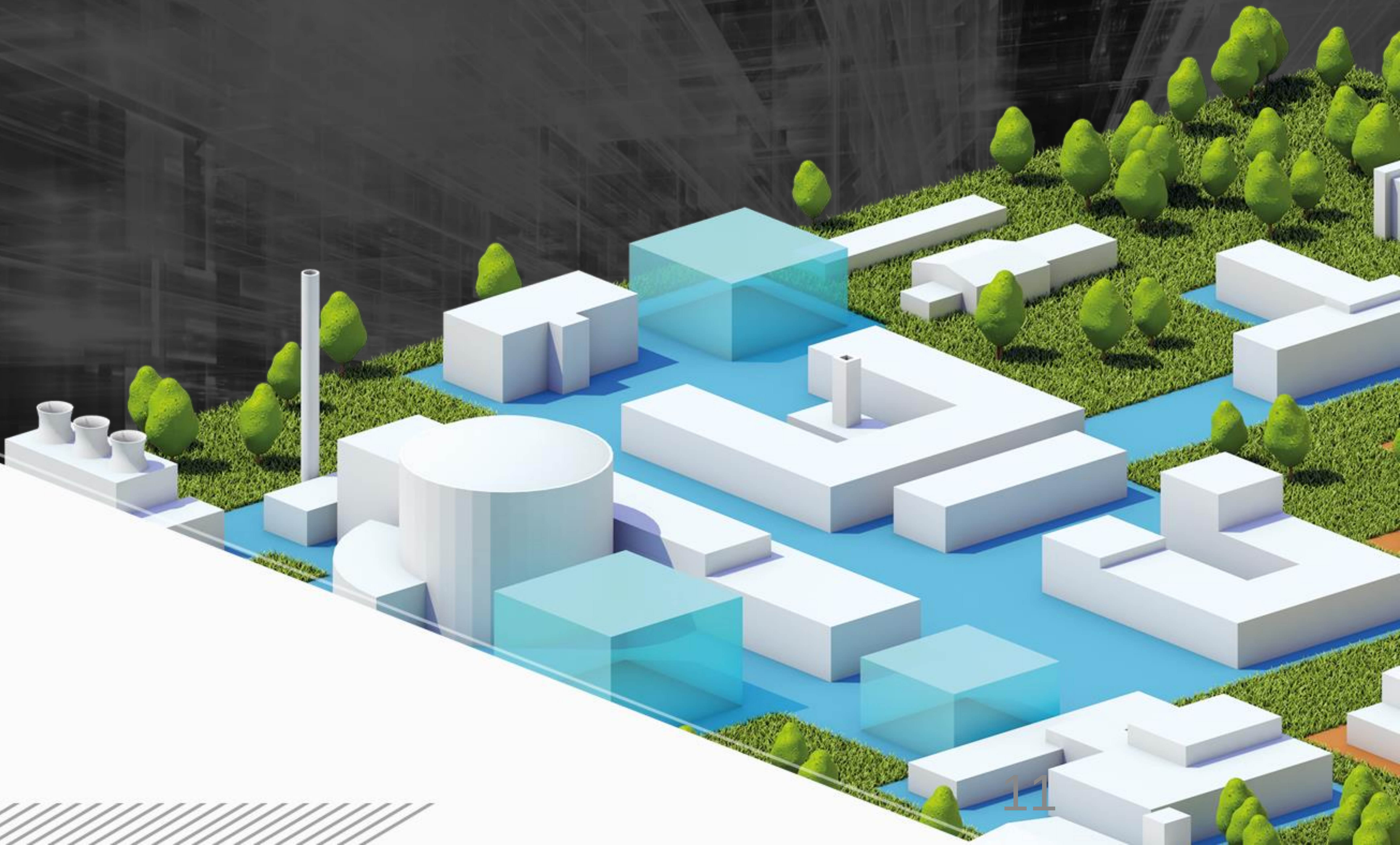
Thank you



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