Scalable Machine Learning for Predicting the Electronic Structure of Matter

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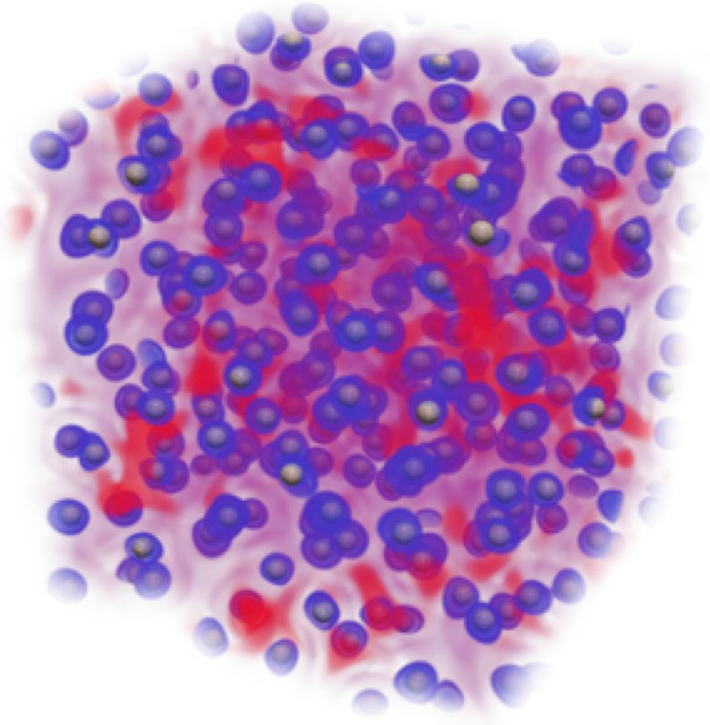

MALA
Materials Learning Algorithms

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Electronic Structure Problem

Non-relativistic Schrödinger equation

$$\hat{H}(\underline{\mathbf{r}}, \underline{\mathbf{R}})\Psi(\underline{\mathbf{r}}, \underline{\mathbf{R}}) = E\Psi(\underline{\mathbf{r}}, \underline{\mathbf{R}})$$

$$\hat{H}(\underline{\mathbf{r}}; \underline{\mathbf{R}}) = \hat{T}_e(\underline{\mathbf{r}}) + \hat{V}_{ee}(\underline{\mathbf{r}}) + \hat{V}_{ei}(\underline{\mathbf{r}}; \underline{\mathbf{R}}) + \hat{V}_{ii}(\underline{\mathbf{R}})$$

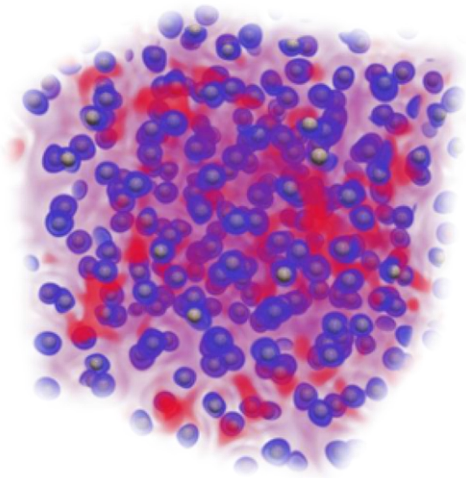
$$\hat{T}_e(\underline{\mathbf{r}}) = \sum_i^{N_e} -\frac{\nabla_i^2}{2}$$

$$\hat{V}_{ee}(\underline{\mathbf{r}}) = \sum_i^{N_e} \sum_{j \neq i}^{N_e} \frac{1}{2} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

$$\hat{V}_{ei}(\underline{\mathbf{r}}; \underline{\mathbf{R}}) = -\sum_i^{N_e} \sum_\alpha^{N_i} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}$$

$$\hat{V}_{ii}(\underline{\mathbf{R}}) = -\sum_\alpha^{N_i} \sum_{\beta \neq \alpha}^{N_i} \frac{1}{2} \frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}$$

Molecular and materials properties



Molecular structure, Crystal structure, Charge density, Cohesive energy, Elastic properties, Vibrational properties, Magnetic order, Dielectric susceptibility, Magnetic susceptibility, Phase transitions, Bond dissociation, Enthalpies of formation, Ionization potential, Electron affinity, Band gaps, Equation of state

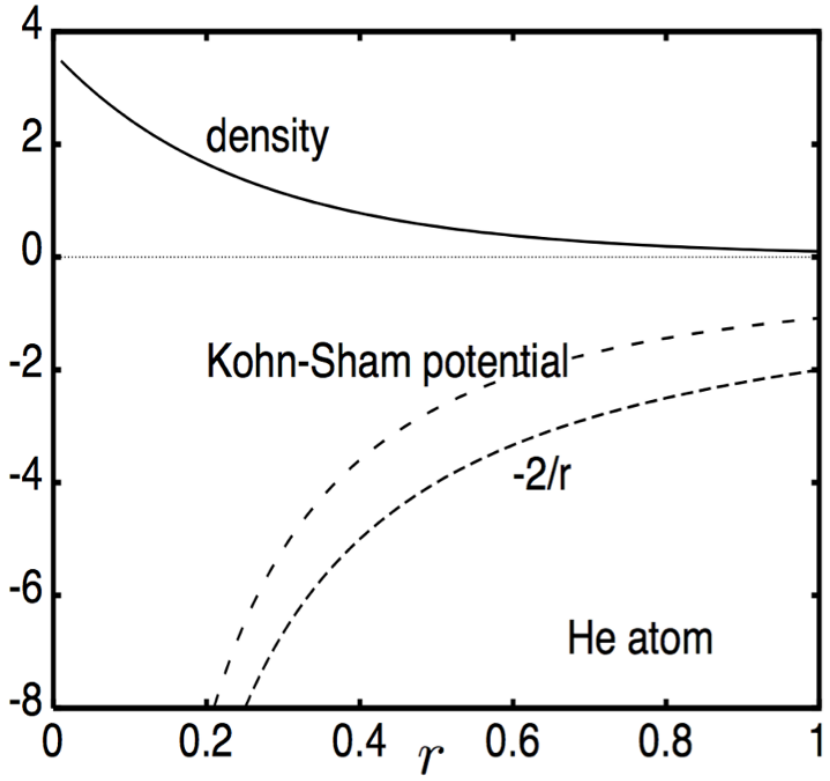
Density Functional Theory

$$\left[-\frac{1}{2}\nabla^2 + v_{\mathrm{S}}(\mathbf{r};\underline{\mathbf{R}})\right]\phi_j(\mathbf{r};\underline{\mathbf{R}}) = \epsilon_j\phi_j(\mathbf{r};\underline{\mathbf{R}})$$

$$v_{\mathrm{S}}(\mathbf{r};\underline{\mathbf{R}}) = \frac{\delta U[n]}{\delta n(\mathbf{r};\underline{\mathbf{R}})} + \frac{\delta E_{\mathrm{XC}}[n]}{\delta n(\mathbf{r};\underline{\mathbf{R}})} + v_{ei}(\mathbf{r};\underline{\mathbf{R}})$$

$$n(\mathbf{r};\underline{\mathbf{R}}) = \sum_j \phi_j^*(\mathbf{r};\underline{\mathbf{R}})\phi_j(\mathbf{r};\underline{\mathbf{R}})$$

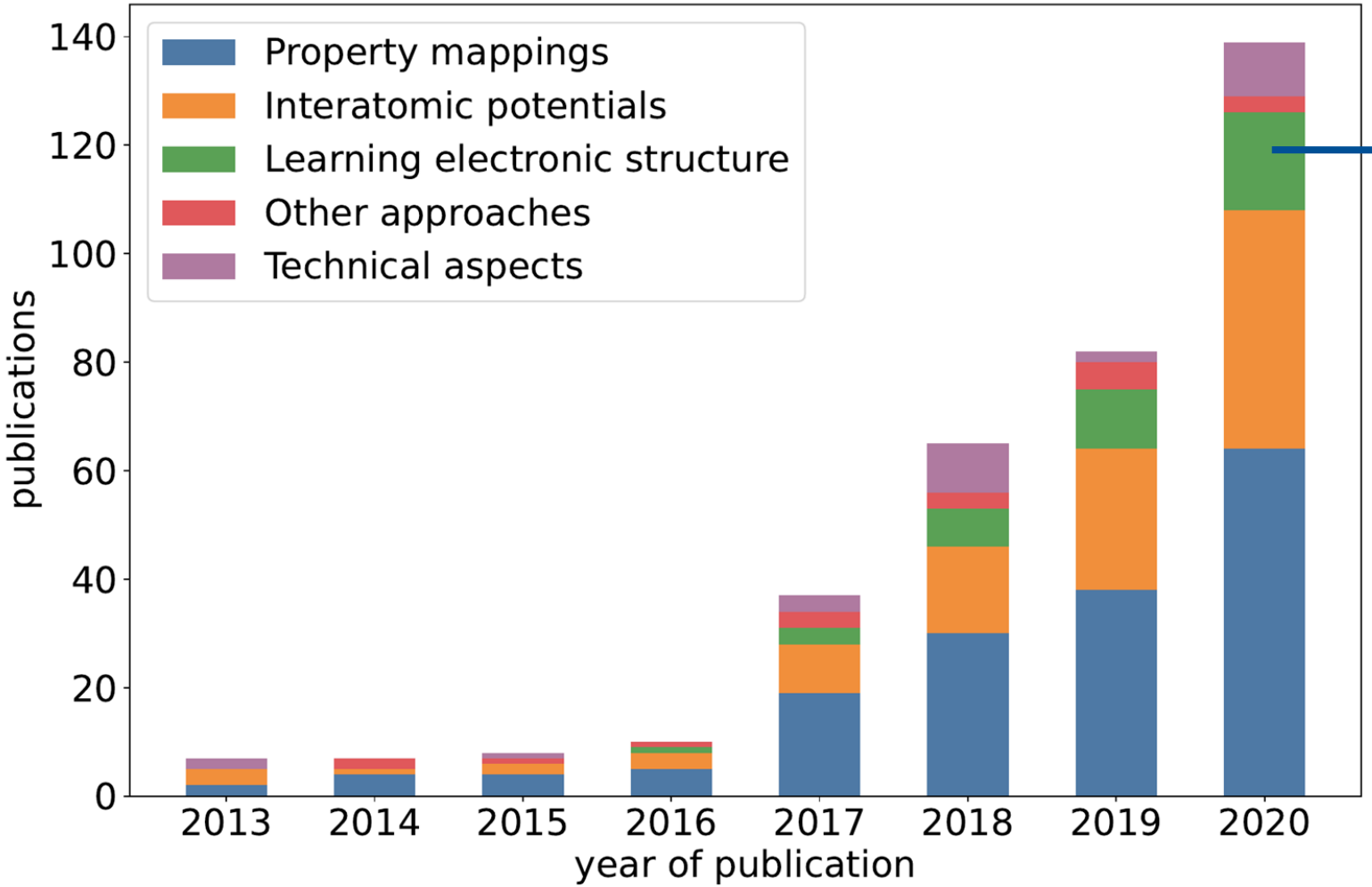
$$E[n] = T_{\mathrm{S}}[n] + U[n] + E_{\mathrm{XC}}[n] + \int d^3r\; n(\mathbf{r};\underline{\mathbf{R}})v_{ei}(\mathbf{r};\underline{\mathbf{R}})$$



K. Burke, „The ABC of DFT“.

Why:

State of the art in combining electronic structure theory with machine learning



Machine learning the electronic structure (this work)

Meta study analyzing 370 research articles

L. Fiedler, K. Shah, M. Bussmann, A. Cangi, Phys. Rev. Mater. 6, 040301 (2022).

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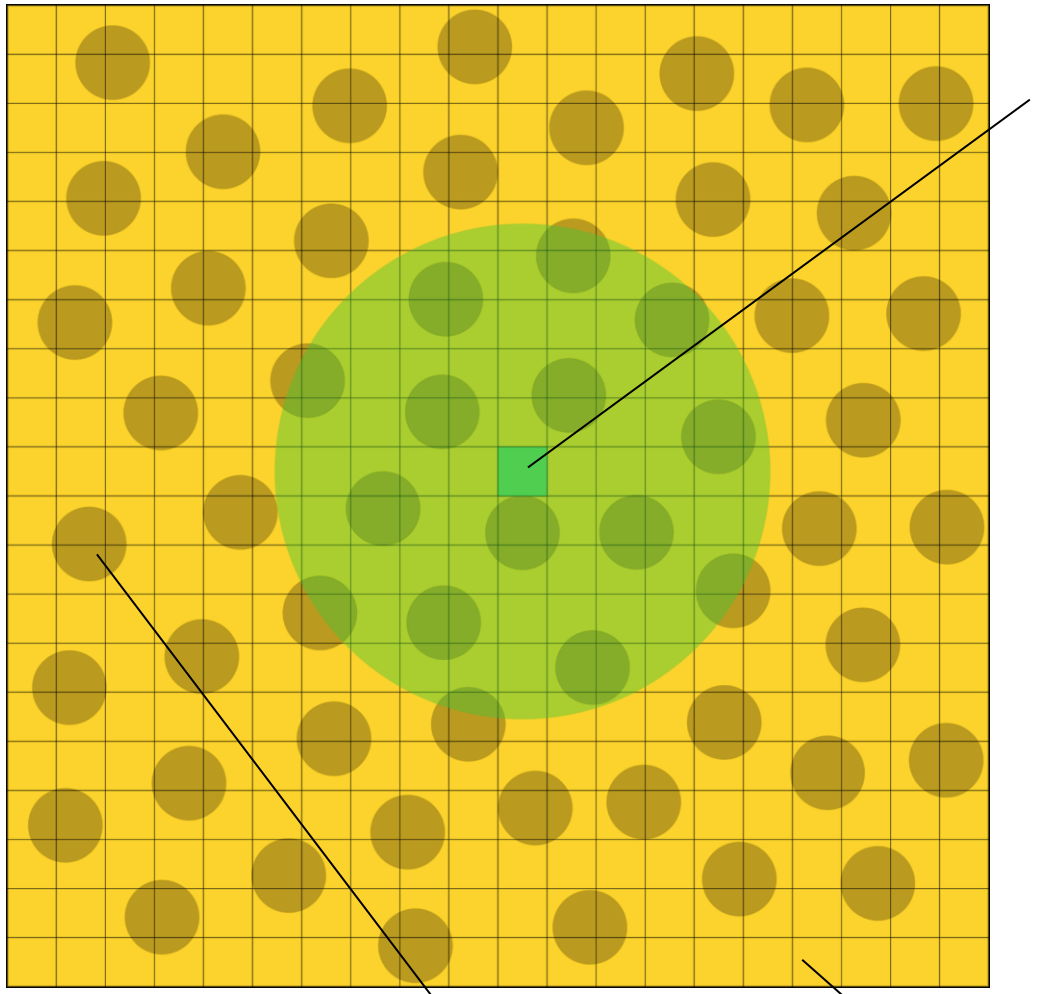
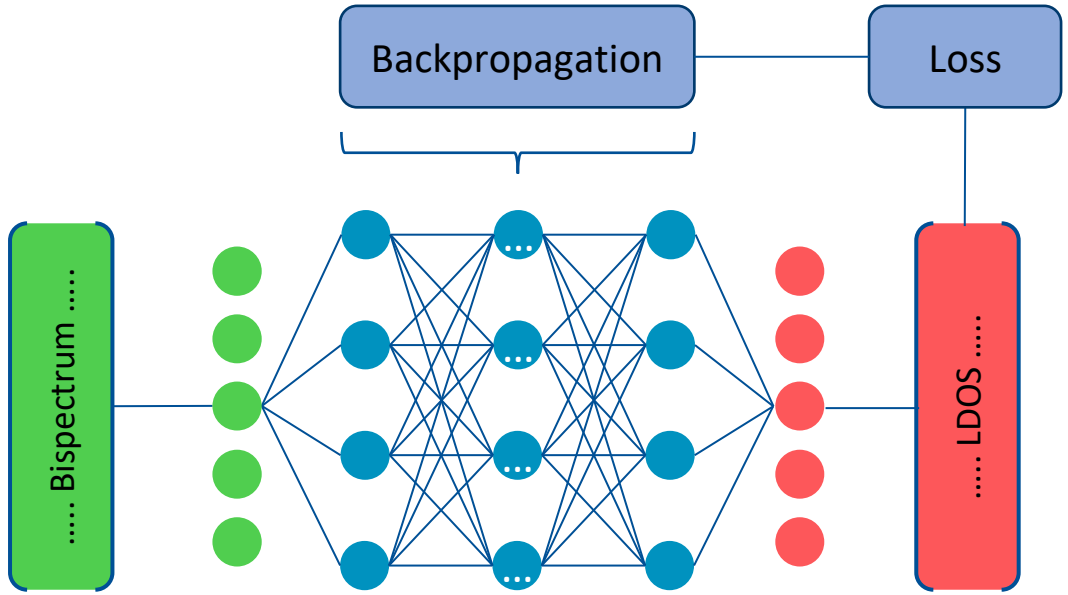
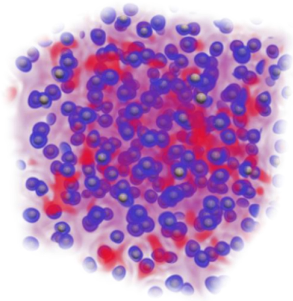
Spatially resolved neural-network model for the local density of states







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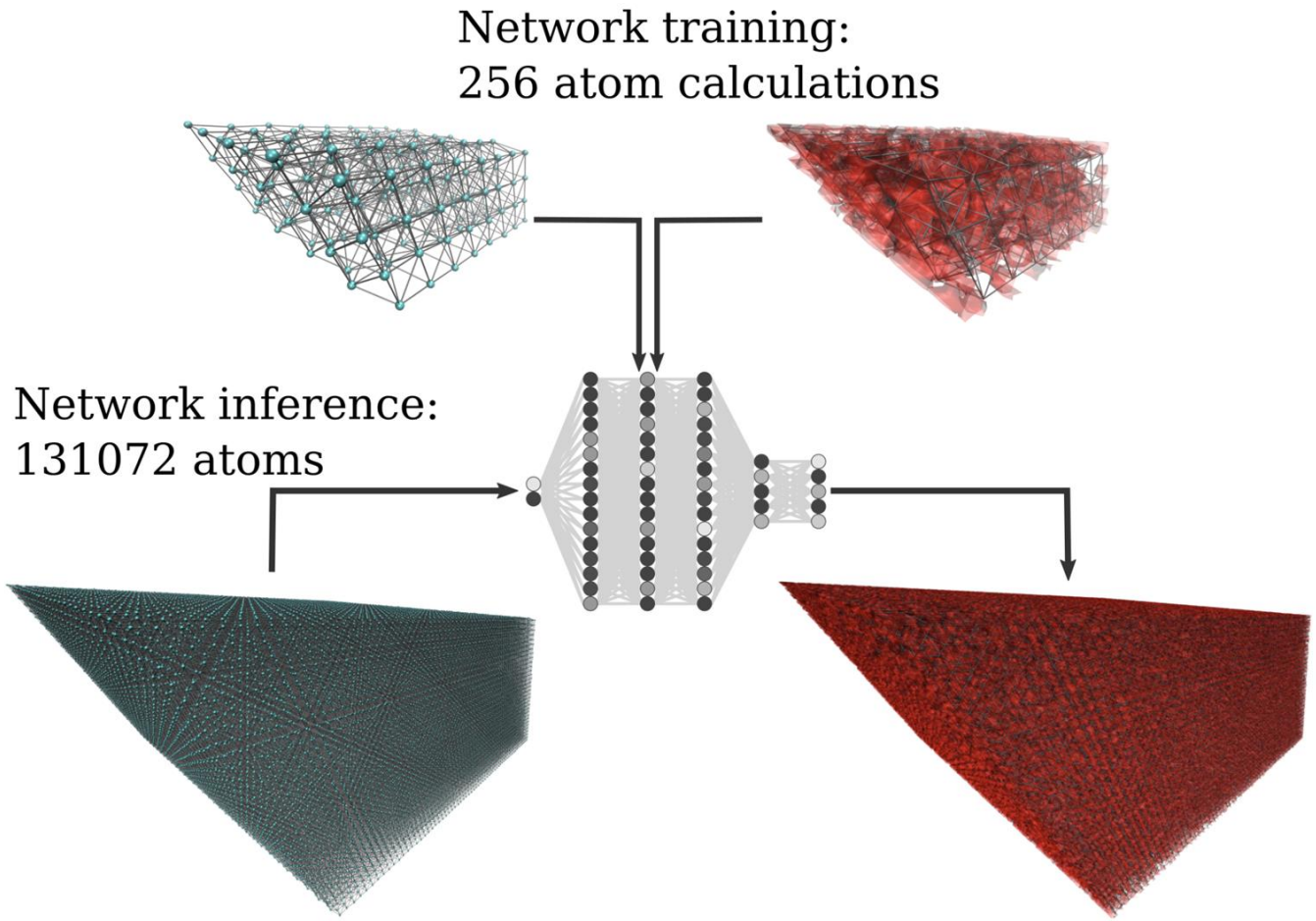
Interpolation across the number of atoms



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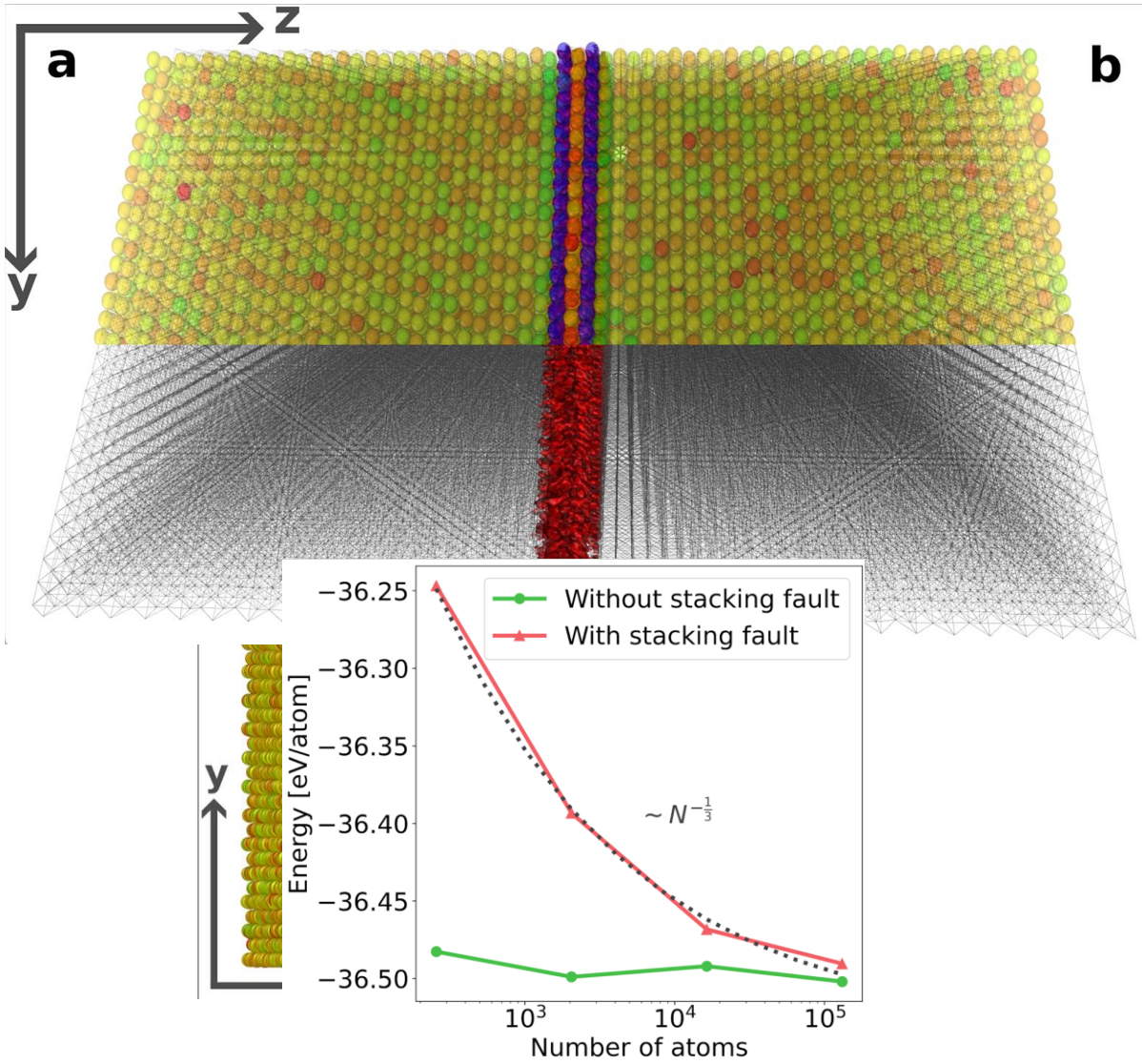
Interpolation across the number of atoms

Example: Stacking fault

Introduce a stacking fault into a slab of Beryllium (change local crystal structure from hcp to fcc).

Predict the electronic structure for this system that contains 131,072 atoms.



MALA USP:

Development goals

Scalability