

MALA background

MALA tutorial

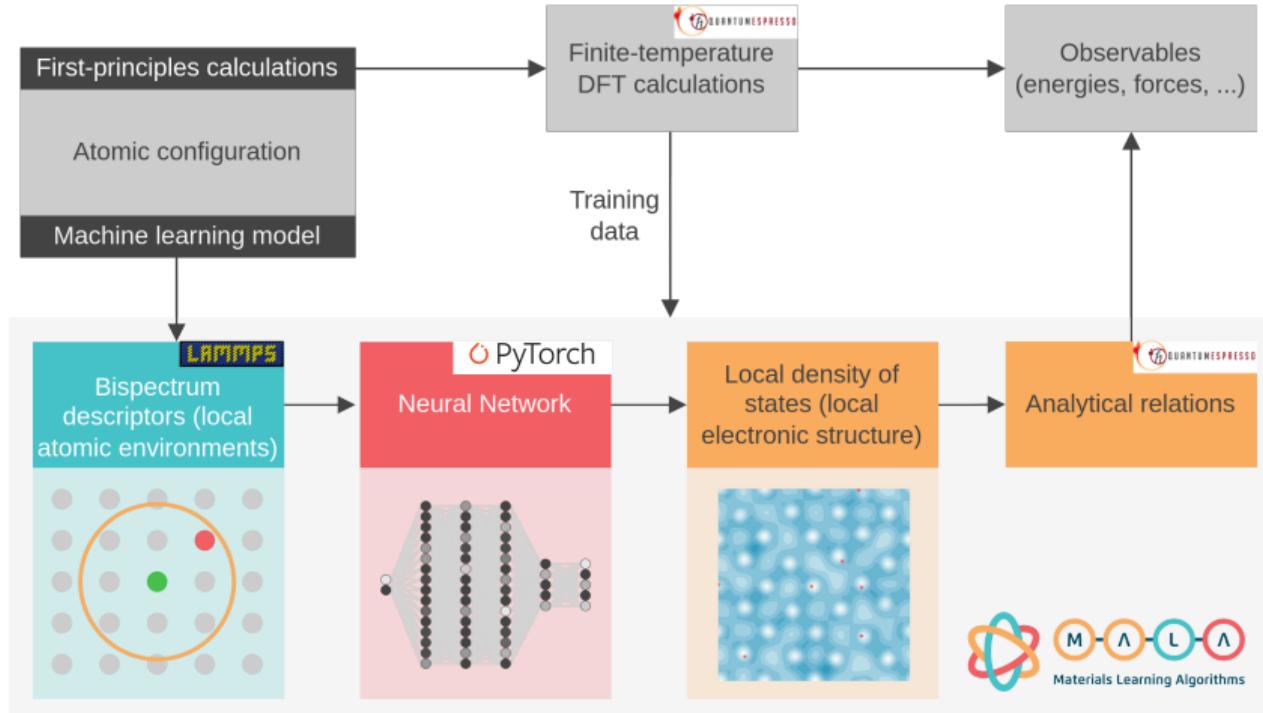
21.03.2022 // Lenz Fiedler



```
mirror_object to mirror
mirror_mod.mirror_object
operation == "MIRROR_X":
    mirror_mod.use_x = True
    mirror_mod.use_y = False
    mirror_mod.use_z = False
    operation == "MIRROR_Y"
    mirror_mod.use_x = False
    mirror_mod.use_y = True
    mirror_mod.use_z = False
    operation == "MIRROR_Z"
    mirror_mod.use_x = False
    mirror_mod.use_y = False
    mirror_mod.use_z = True
```



MALA workflow



Relevant equations

$$A[n] = A[n, \phi_j[n]] = T_S[\phi_j[n]] - k_B \tau S_S[\phi_j[n]] + E_H[n] + E_{XC}[n] + E^{ei}[n]$$

Relevant equations

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$$d(\epsilon, \mathbf{r}) = \sum_j |\phi_j(\mathbf{r})|^2 \delta(\epsilon - \epsilon_j)$$

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$$d(\epsilon, \mathbf{r}) = \sum_j |\phi_j(\mathbf{r})|^2 \delta(\epsilon - \epsilon_j)$$

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$$D(\epsilon) = \int d\mathbf{r} d(\epsilon, \mathbf{r})$$

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$$A[n] = A[n[d], D[d]] = E_b[D[d]] - k_B \tau S_S[D[d]] - E_H[n[d]] + E_{XC}[n[d]] - \int d\mathbf{r} v_{XC}(\mathbf{r}) n[d](\mathbf{r})$$

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$$\tilde{d}(\epsilon, \mathbf{r}) = M(B(J, \mathbf{r}))$$

- Accelerating finite-temperature Kohn-Sham density functional theory with deep neural networks, J. A. Ellis, *et al* 2021 *Phys. Rev. B* 104, 035120

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- Training-free hyperparameter optimization of neural networks for electronic structures in matter, L. Fiedler *et al* 2022 *Mach. Learn.: Sci. Technol.* **3** 045008

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- Predicting electronic structures at any length scale with machine learning, L. Fiedler *et al*, publication pending, *arXiv:2210.11343*

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- Check MALA out on GitHub: <https://github.com/mala-project>

MALA cooperation partners



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