

# MALA background

## MALA tutorial

21.03.2022 // Lenz Fiedler



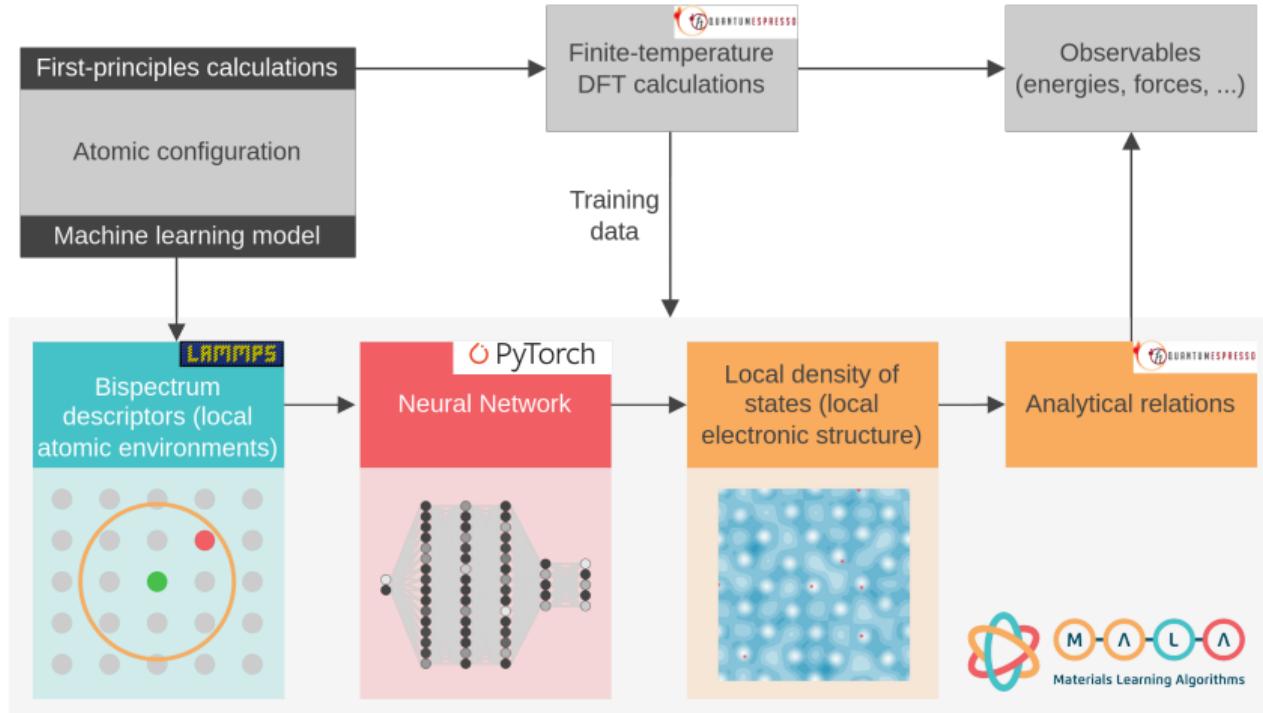
```
mirror_object to mirror
mirror_mod.mirror_object
operation == "MIRROR_X":
    mirror_mod.use_x = True
    mirror_mod.use_y = False
    mirror_mod.use_z = False
    operation == "MIRROR_Y"
    mirror_mod.use_x = False
    mirror_mod.use_y = True
    mirror_mod.use_z = False
    operation == "MIRROR_Z"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



# Contents



# MALA workflow



## Relevant equations

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

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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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- 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



Sandia  
National  
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