Active Learning of Physics Aware Potentials for Nanostructured Systems: Application in Gas Sensing

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Overall Goal

- ❑ Use atomic scale simulations (Molecular Dynamics) to facilitate understanding and the design of novel materials like gas sensing devices.
- ❑ To simulate any atomic scale system classically via Molecular Dynamics (MD) the potential energy is needed $H(\boldsymbol{r},\boldsymbol{v}) = KE(\boldsymbol{v}) + U(\boldsymbol{r}) + \cdots$

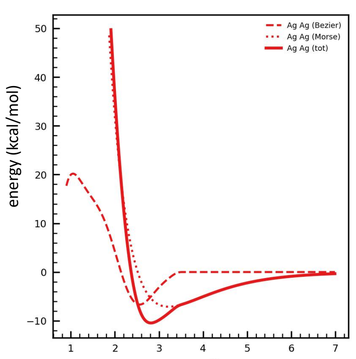
Main Challenges

- ❑ Nanoscale gas sensing devices are characterized by rough undercoordinated gas/solid interfaces.
- ❑ And these interfaces by complex quantum scale interactions.
- ❑ Develop an accurate and computationally efficient **classical model** describing the **different physicochemical interactions.**

1. Sample Density Functional Theory (DFT) data

Quantum scale → **Atomic scale**

2. Fit a classical Physics Aware model



$$U_{class}(\mathbf{r}) = U_B(\mathbf{r}) + U_{PW}(\mathbf{r}) + U_E(\mathbf{r})$$

$$U_B(\mathbf{r}) = \sum_b f_b(r_b) + \sum_a f_a(\theta_a) + \sum_d f_d(\phi_d)$$

$$U_{PW}(\mathbf{r}) = \sum_{i<j} f_{pw}(r_{ij})$$

$$U_E(\mathbf{r}) = \sum_{i,\beta\in B_i} f_e\left(\rho^i_{\alpha\beta}\right) \qquad \rho^i_{\alpha\beta} = \sum_{j\in\beta} \varphi(r_{ij})$$

coordination

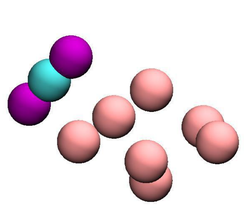
Incorporating physics awareness and flexibility

Curves f are parameterized as a superposition of

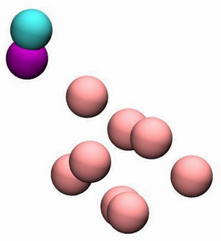
- ➢ **semi-empirical** potentials, like Morse, and
- ➢ smooth curves of arbitrary shape (**Bezier polynomials**)

Promising for gas sensing applications!

- **cohesive forces (undercoordinated systems, different than the bulk)**
- **gas physisorption (up to 9 kcal/mol for co2)**
- **gas chemisorption (Very strong interactions >30 kcal/mol, exchange of electrons)**



Ag_7CO_2



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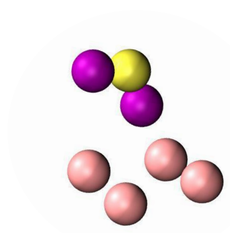
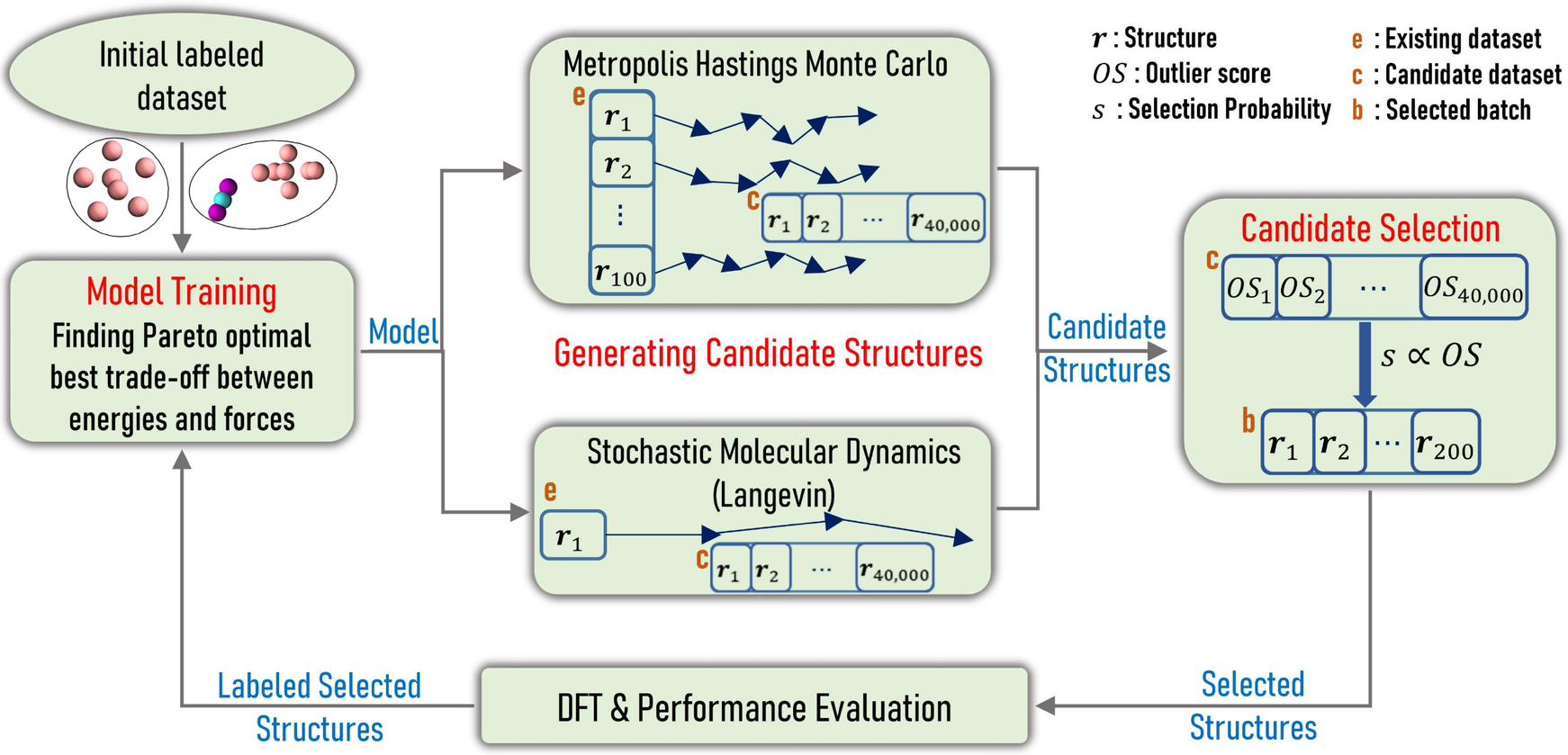
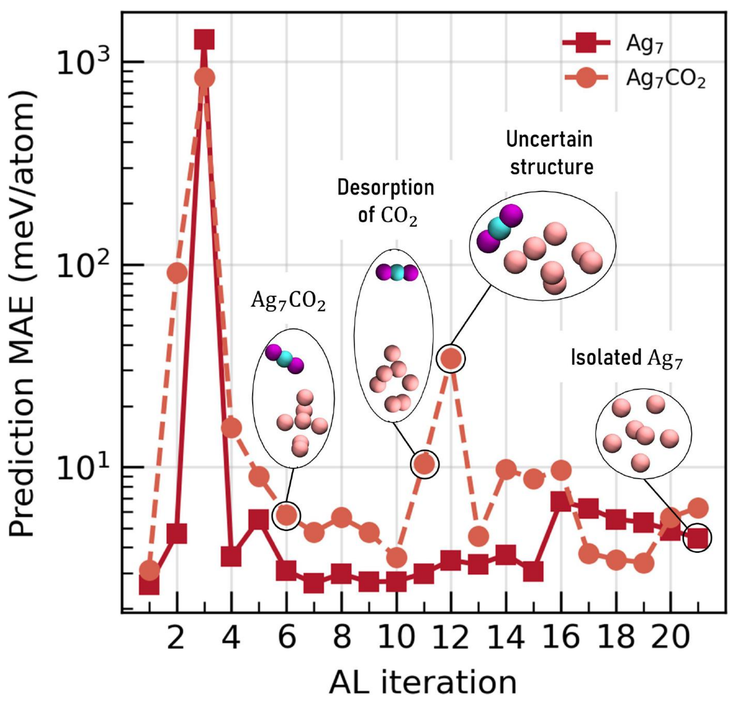


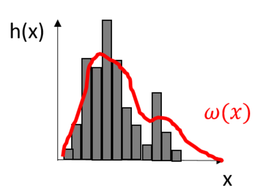
Ag_4SO_2

Solution: Active Learning (AL) of Physics Aware Models

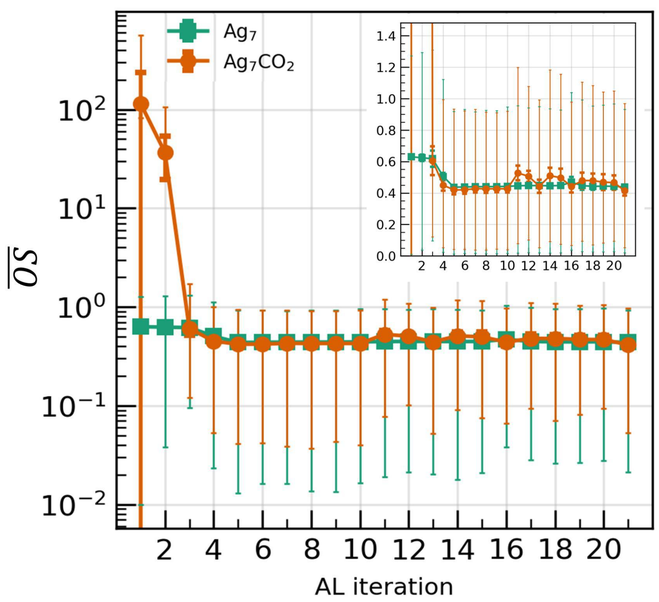
- ❑ Actively explore the Potential Energy Surface (PES) at the quantum scale via DFT calculations and train classical atomic scale **physics aware machine learning models**.







$$OS(\mathbf{d}) = \left(\frac{1}{m}\sum_{i=1}^{m}(1-\overline{\omega}(d_i))^3\right)^{1/3}$$



References

- Mohammadi, Mohsen Doust, et al. "Adsorption of air pollutants onto silver and gold atomic clusters: DFT and PNO-LCCSD-F12 calculations." *RSC advances* 13.26 (2023): 18014-18024.
- **Patsalidis et. al. "Active Learning of Atomic Size Gas/Solid Potential Energy Surfaces via Physics Aware Models" (submitted)**

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