Massachusetts Institute of Technology

Exploring materials surfaces with deep learning for CO_2 reduction

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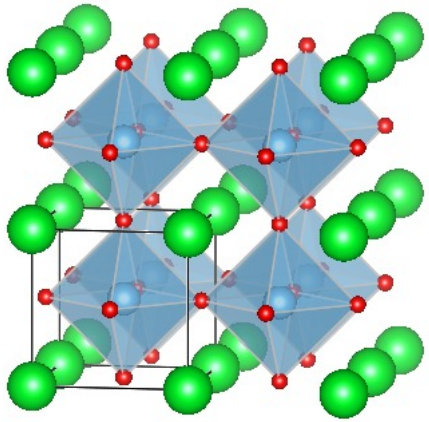
GraphEx Symposium

17 May 2022

Metal oxides for CO_2 reduction

1. It is critical to mitigate atmospheric CO_2 increase to avoid a climate crisis.
2. Metal oxides are especially promising for CO_2 air capture.
3. Goal: study the surface of perovskite oxide strontium titanate ($SrTiO_3$).

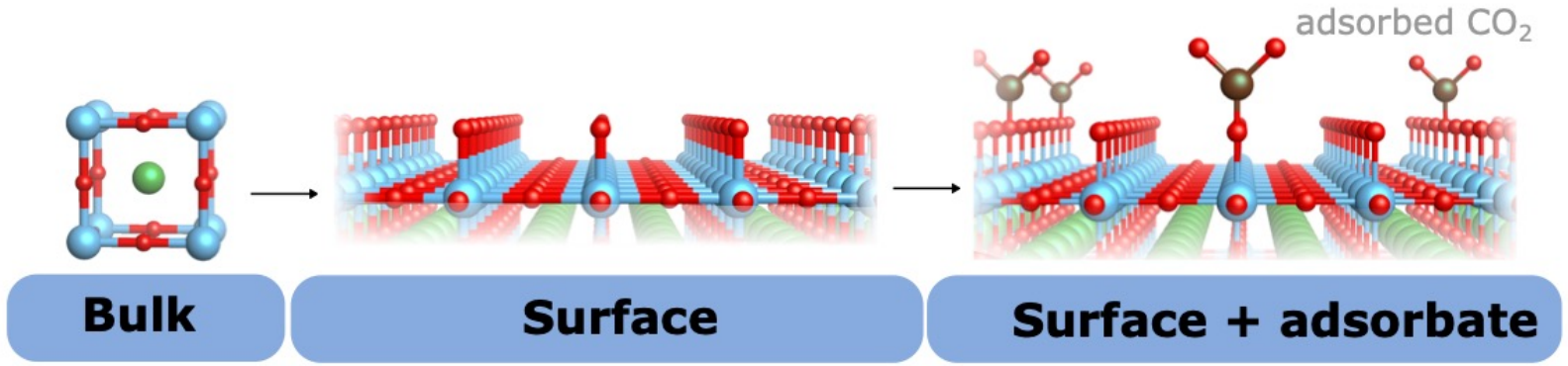
$SrTiO_3$ crystal
(https://geology.com/gemstones/strontium-titanate/)

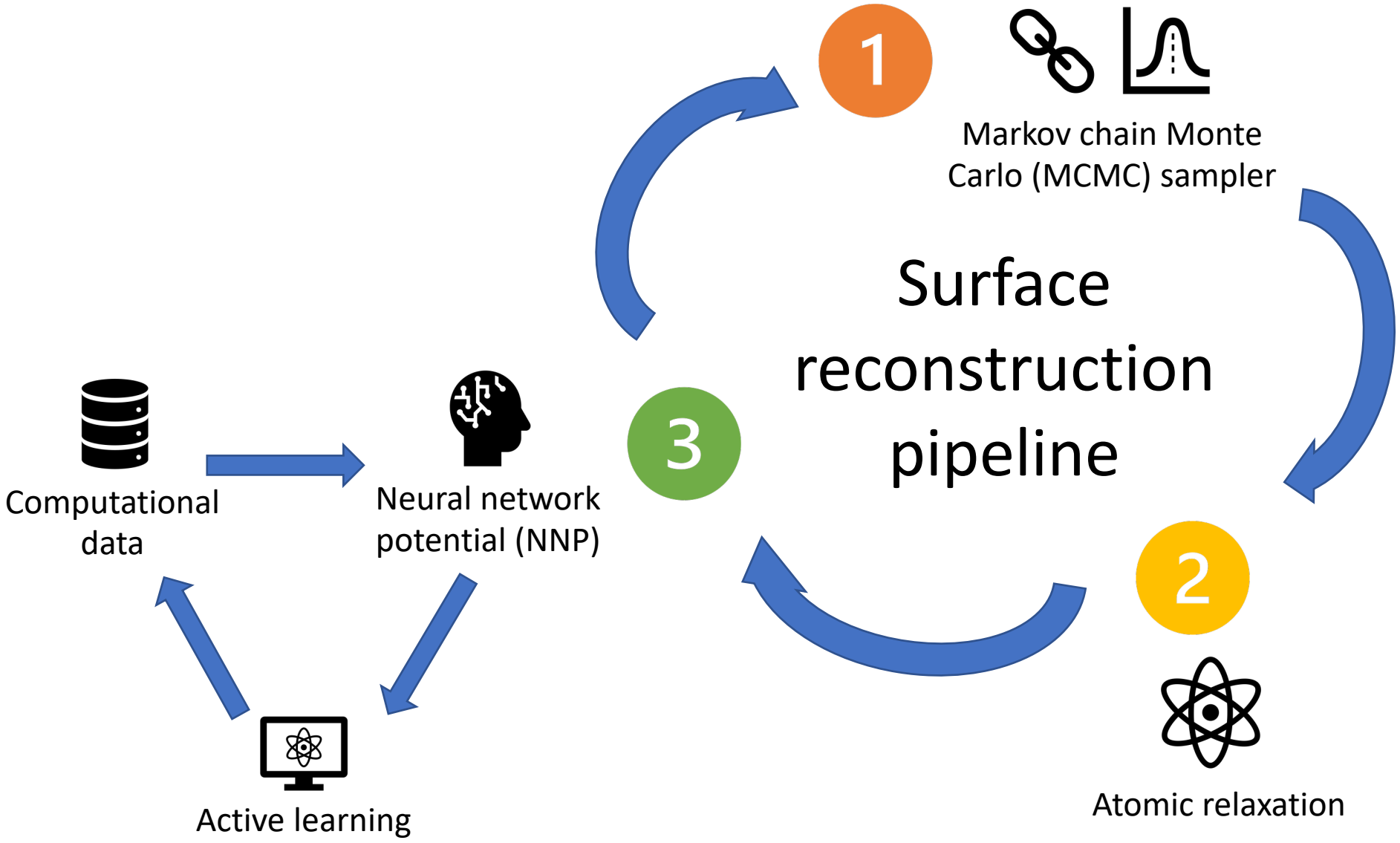


$SrTiO_3$ crystal structure
(https://commons.wikimedia.org/wiki/File:Cubic_SrTiO3.png)

Why study materials surfaces?

1. Materials surfaces often differ significantly from the bulk in both structure and composition.
2. These surface reconstructions are key because chemical reactions take place on the surface.
3. We need to understand the thermodynamics of the material surface.




1
Markov chain Monte Carlo (MCMC) sampler
Surface reconstruction pipeline
2
Atomic relaxation
3
Neural network potential (NNP)
Computational data
Active learning

Acknowledgements

- MIT: Prof. Rafael Gómez-Bombarelli, James Damewood, Jaclyn Lunger
- MIT Lincoln Lab: Lin Li (Program Manager), Nathan Frey

Funding:

ChemE

NSF GRADUATE RESEARCH FELLOWSHIP PROGRAM

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship Program under Grant No. 1745302. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.