# Finding Reaction Pathways with optimal atomic index mappings

Stefan Goedecker[a]

[a] *Department of Physics, University of Basel*
stefan.goedecker@unibas.ch

Finding complex reaction and transformation pathways, involving many intermediate states, is in general not possible on the DFT level with existing simulation methods due to the very large number of required energy and force evaluations. This is due to a large extent to the fact that for complex reactions, it is not possible to determine which atom in the educt is mapped onto which atom in the product. Trying out all possible atomic index mappings is not feasible because of the factorial increase in the number of possible mappings. By using a penalty function that is invariant under index permutations, we can bias the potential energy surface in such a way that it obtains the characteristics of a structure seeker whose global minimum is the product. By performing a Minima Hopping based global optimization on this biased potential energy surface we can rapidly find intermediate states that lead into the global minimum. Based on this information we can then extract the full reaction pathway. We first demonstrate for a benchmark system, namely $LJ_{38}$ that our method allows to preferentially find intermediate states that are relevant for the lowest energy reaction pathway and that we therefore need a much smaller number of intermediate states than previous methods to find the lowest energy reaction pathway. Finally we apply the method to two real systems, $C_{60}$ and $C_{20}H_{20}$ and show that the found reaction pathway contains valuable information on how the system can be synthesized.

## References

Deb Sankar De, Marco Krummenacher, Bastian Schaefer, Stefan Goedecker: " Finding reaction pathways with optimal atomic index mappings", arXiv:1906.06077