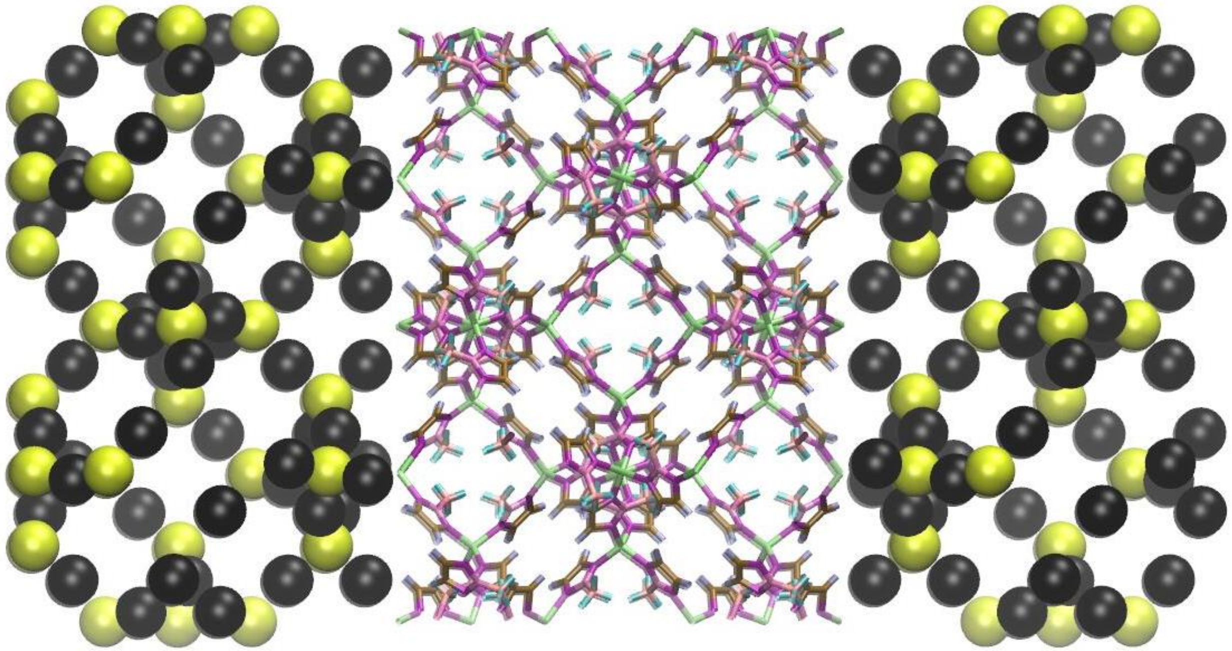
Development and implementation of hybrid atomistic/coarse grained modeling applied to complex interfaces



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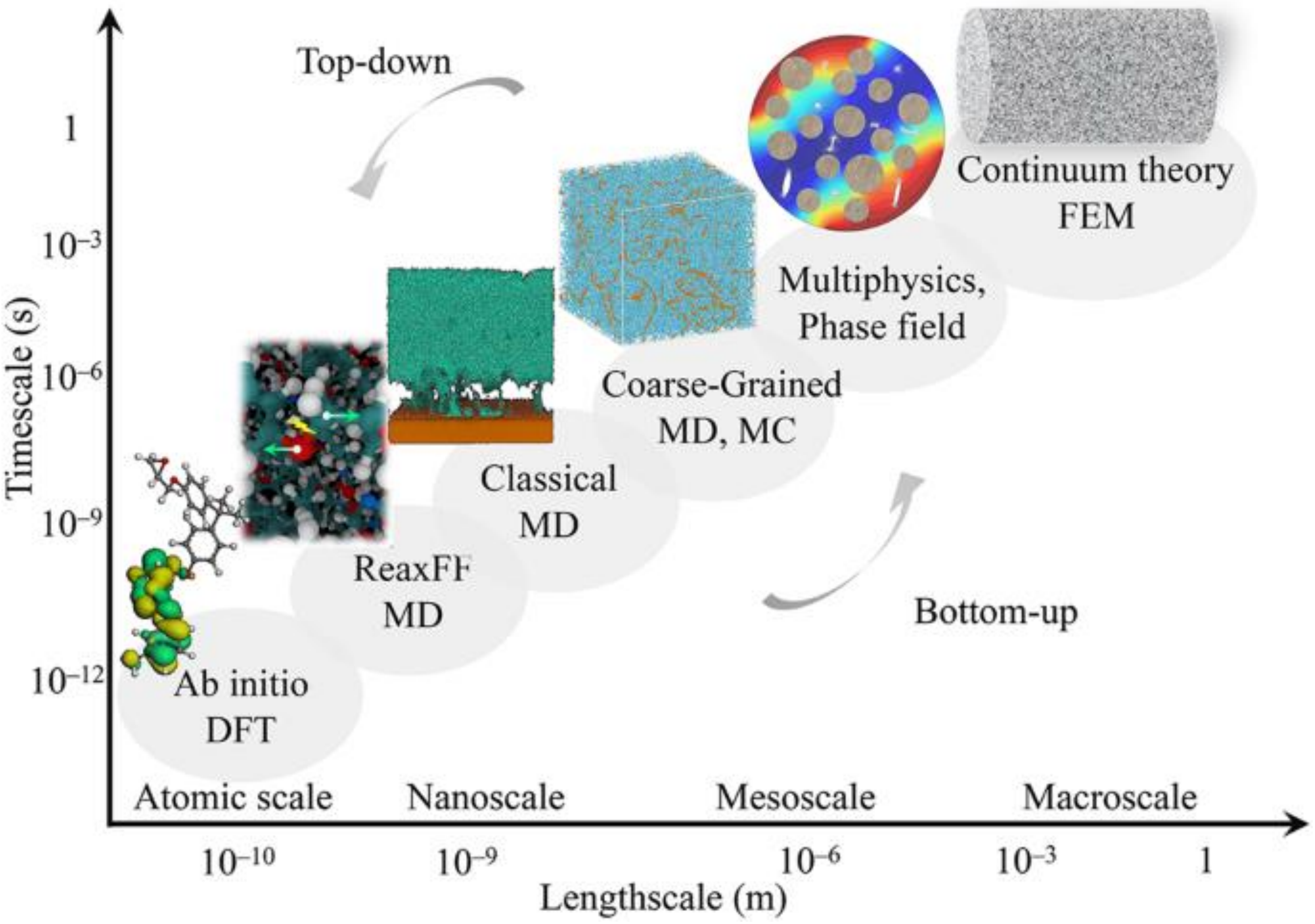
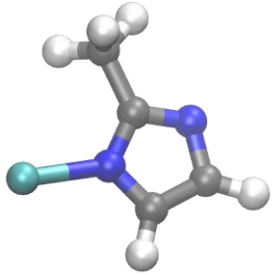
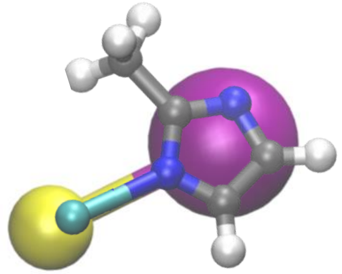


Lin, K., Wang, Z. *Commun Mater* 4, 66 (2023).

All atom scheme

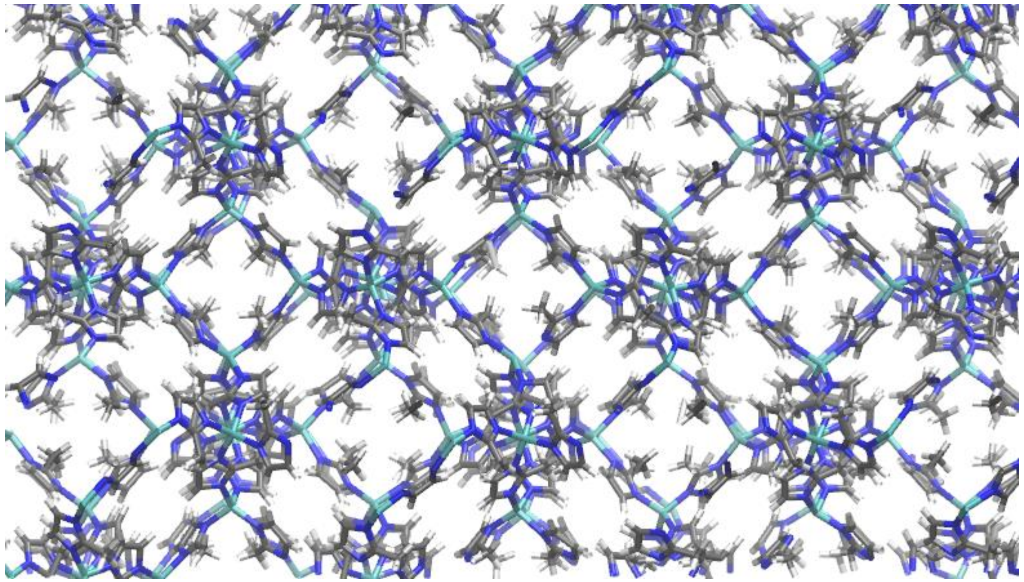


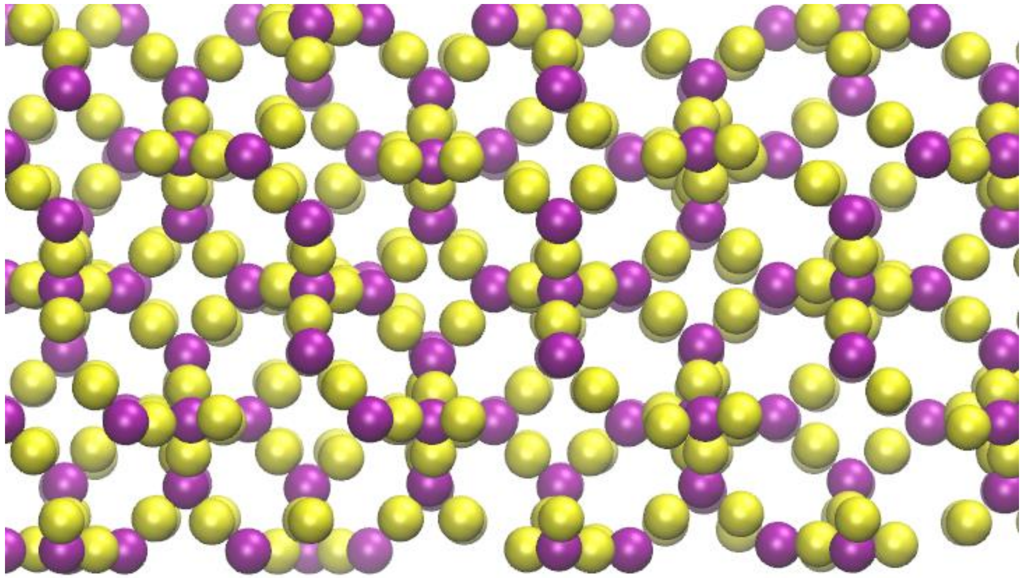
Coarse grained scheme



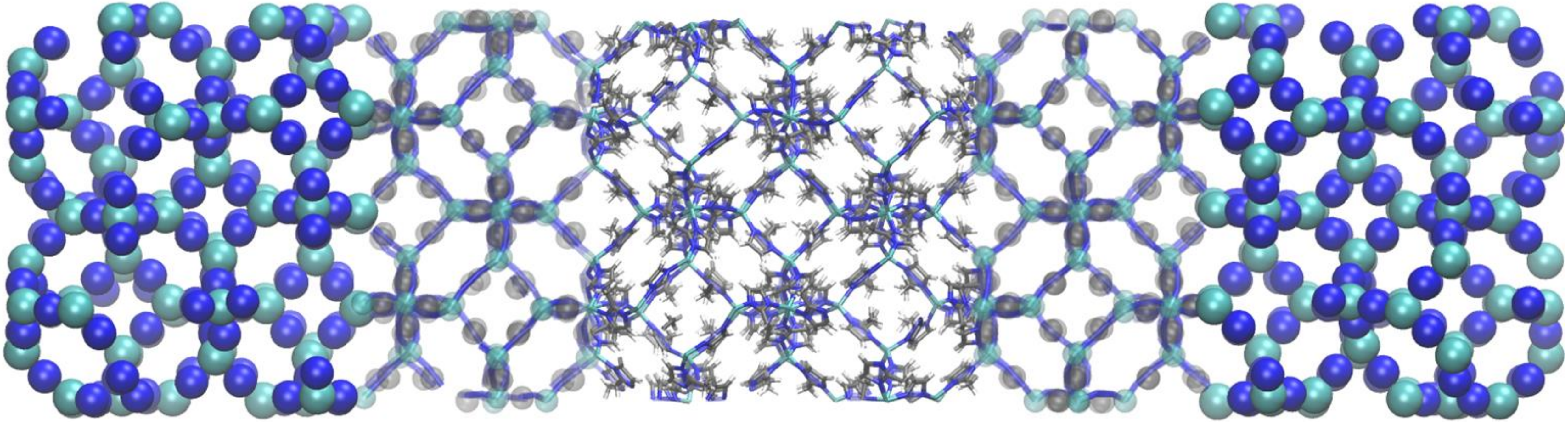
Metal-organic framework: ZIF-8

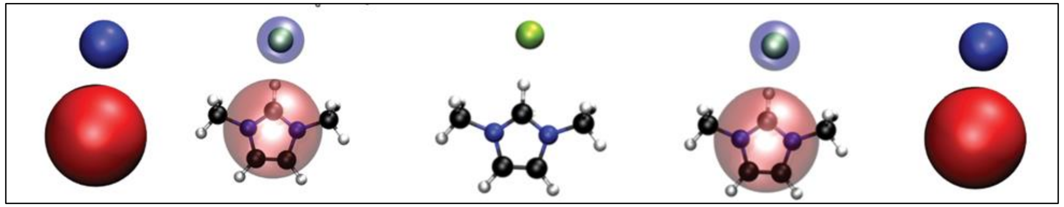
Zn^{2+} + 2(2-methyl imidazolate^{-}) $\longrightarrow$ Zn(2-methyl imidazolate)$_2$

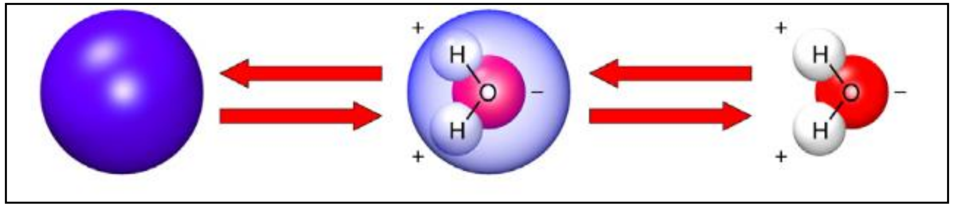


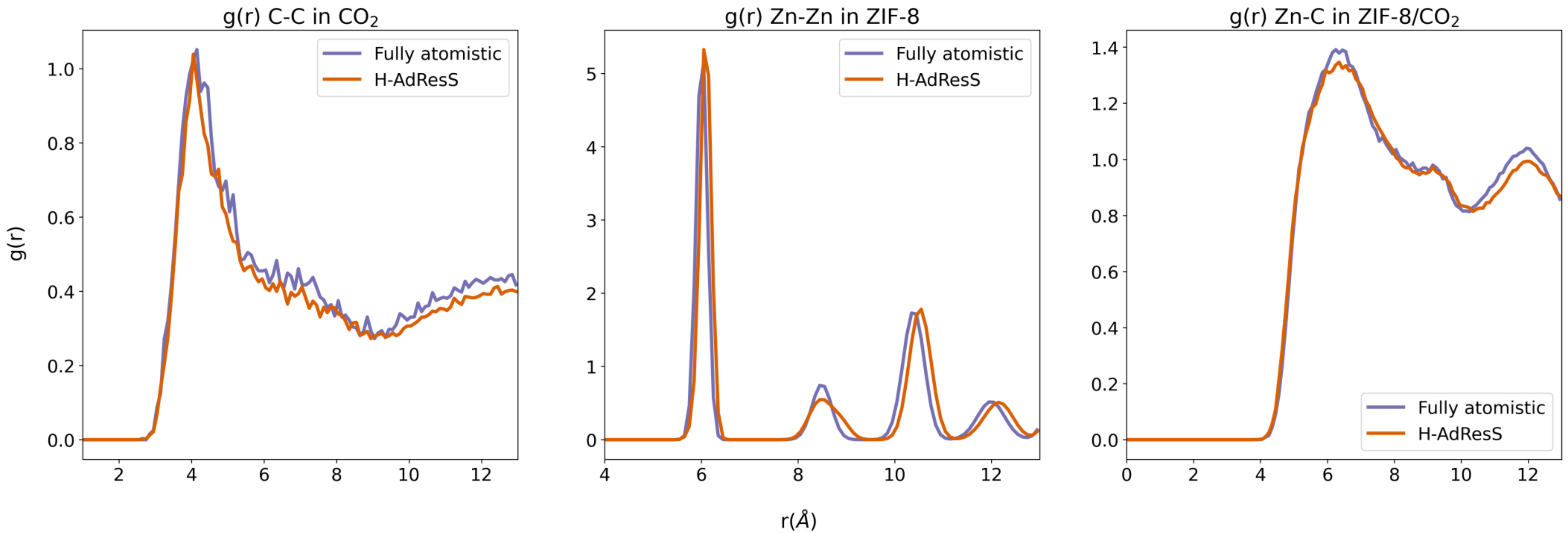


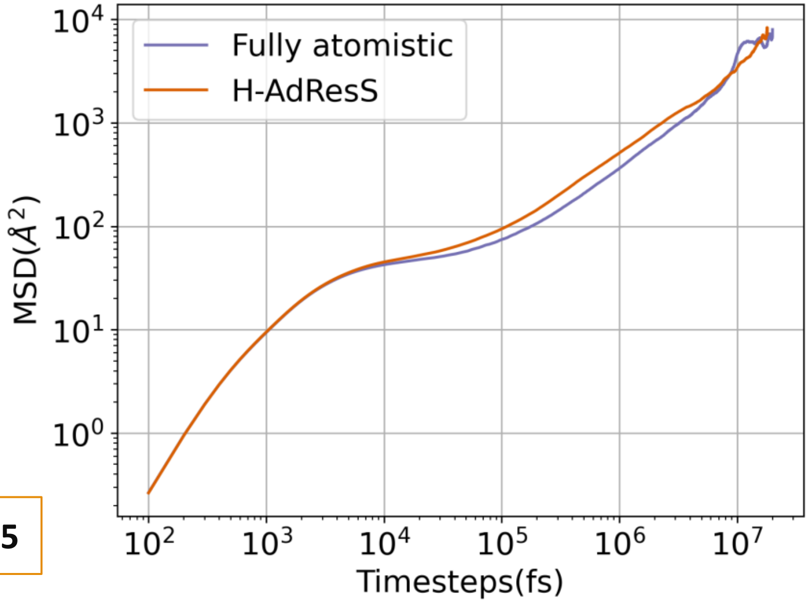
Solution ?

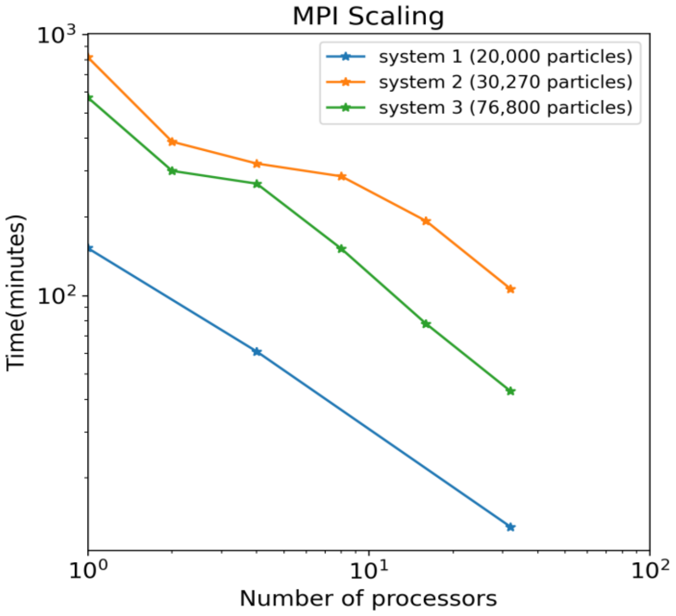


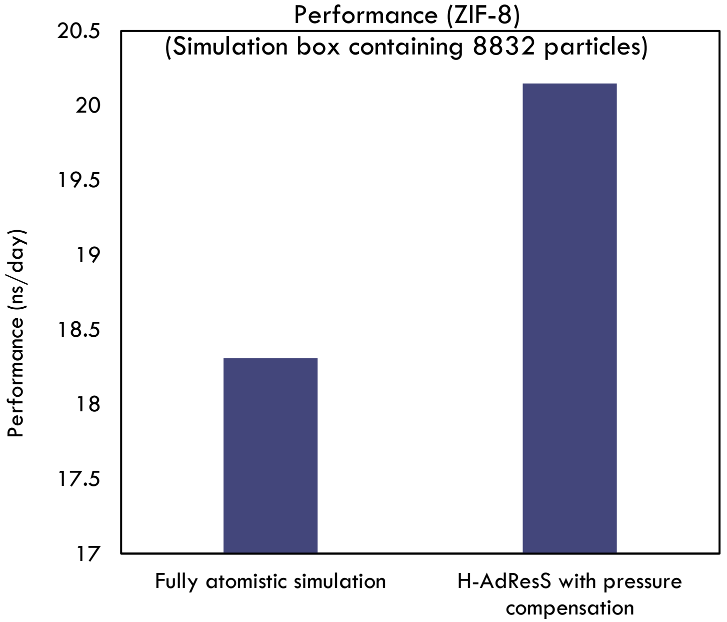




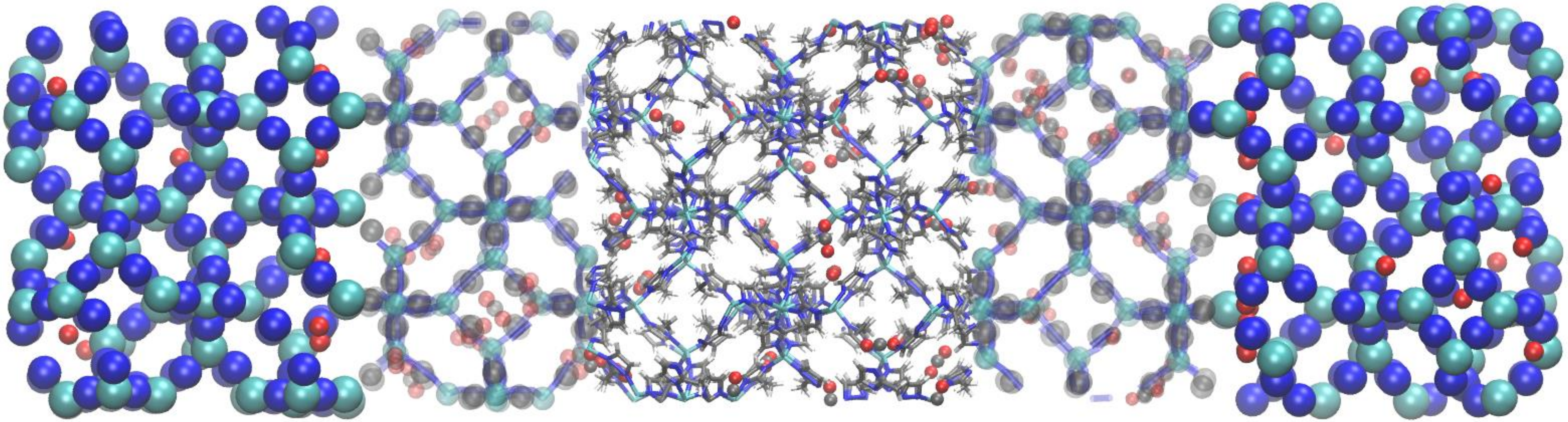

g(r) C-C in CO_2
g(r) Zn-Zn in ZIF-8
g(r) Zn-C in ZIF-8/CO_2
Fully atomistic
H-AdResS
g(r)
r(Å)


Fully atomistic
H-AdResS
MSD($Å^2$)
Timesteps(fs)


MPI Scaling
system 1 (20,000 particles)
system 2 (30,270 particles)
system 3 (76,800 particles)
Time(minutes)
Number of processors


Performance (ZIF-8)
(Simulation box containing 8832 particles)
Performance (ns/day)
Fully atomistic simulation
H-AdResS with pressure compensation

Please do visit my poster!



CONTACT

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