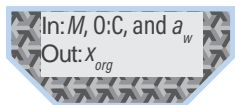


Inputs are a_w , $C_j^{g+\Sigma\pi}$, C_j^{sat} , and chemical information.

Low fidelity
average molecule functionality,
 M_{avg} , O:C_{avg}, (H:C_{avg})

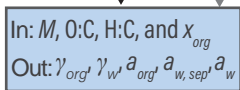
High fidelity
 j^{th} molecule functionality,
 M_j , O:C_j, (H:C_j)

BAT
neural network



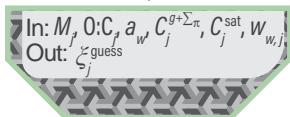
0.13 ms

BAT evaluation
with optional a_w
refinement loop.



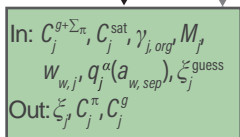
0.58 ms

VBS
neural network



2.8 ms

VBS+BAT evaluation
with equilibrium
solver.



10 ms