pylj: an open-source Python library for teaching the interaction between molecular simulation and scattering

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outline

why?
  molecular dynamics simulation are becoming popular in scattering analysis
what?
  tools to show molecular dynamics simulation and how scattering can be calculated from it
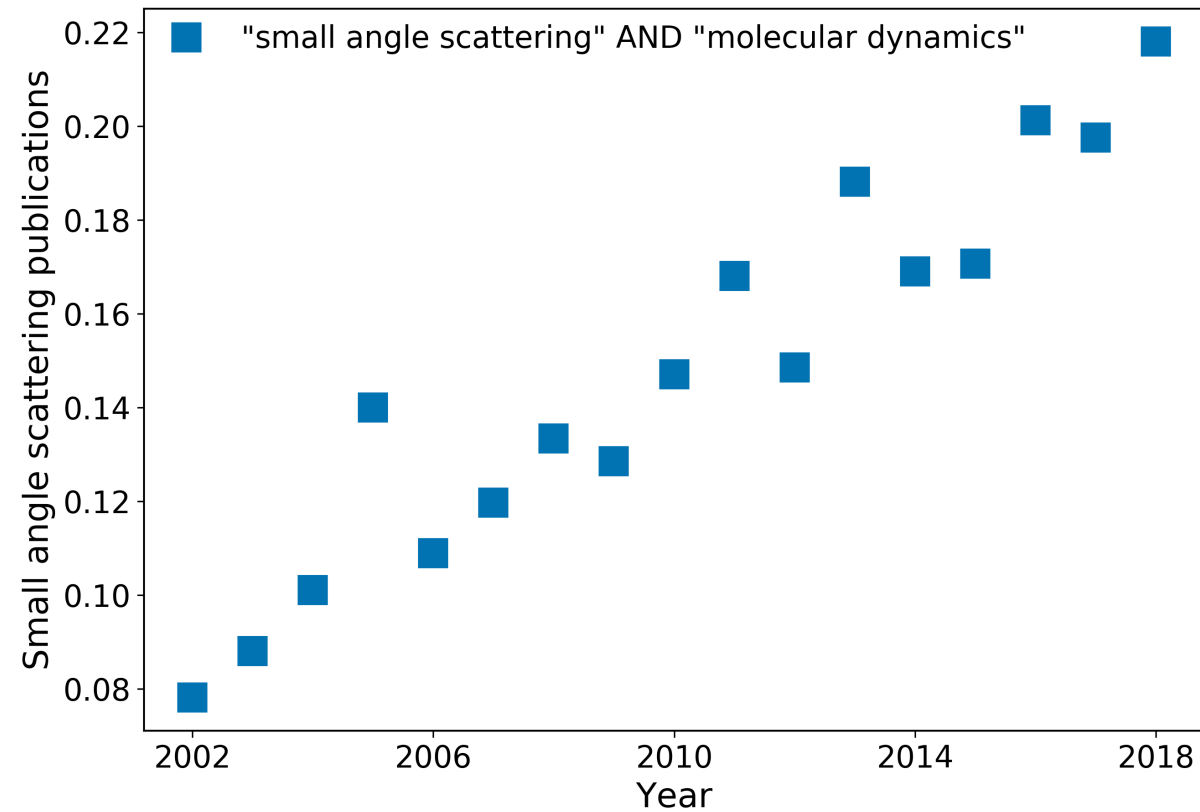**how?**
  pylj

why?

why does classical simulation matter?

simulation is informing our analysis

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simulation is a black box for many

- undergraduates are really introduced to classical simulation in detail
- experimentalists often use tools like waxsis and sassie without understanding what is happening

bring modeling to the masses

@ Bath

- computational chemistry labs from first year
- computational chemistry lectures from second year
- continued to late undergraduate level

# bring modeling to the masses

@ ISIS neutron training course

- half-day introduction to molecular dynamics
- demonstrate theory and show application in neutron science

how?

how can we introduce simulation?

pylj

- open-source, python library to engage students in atomistic simulation
- MIT licence; source code available on GitHub
- paper in *Journal of Open-Source Education*, 1(2), 19. DOI: 10.21105/jose.00019
- particularly useful to show the interaction between simulation and scattering

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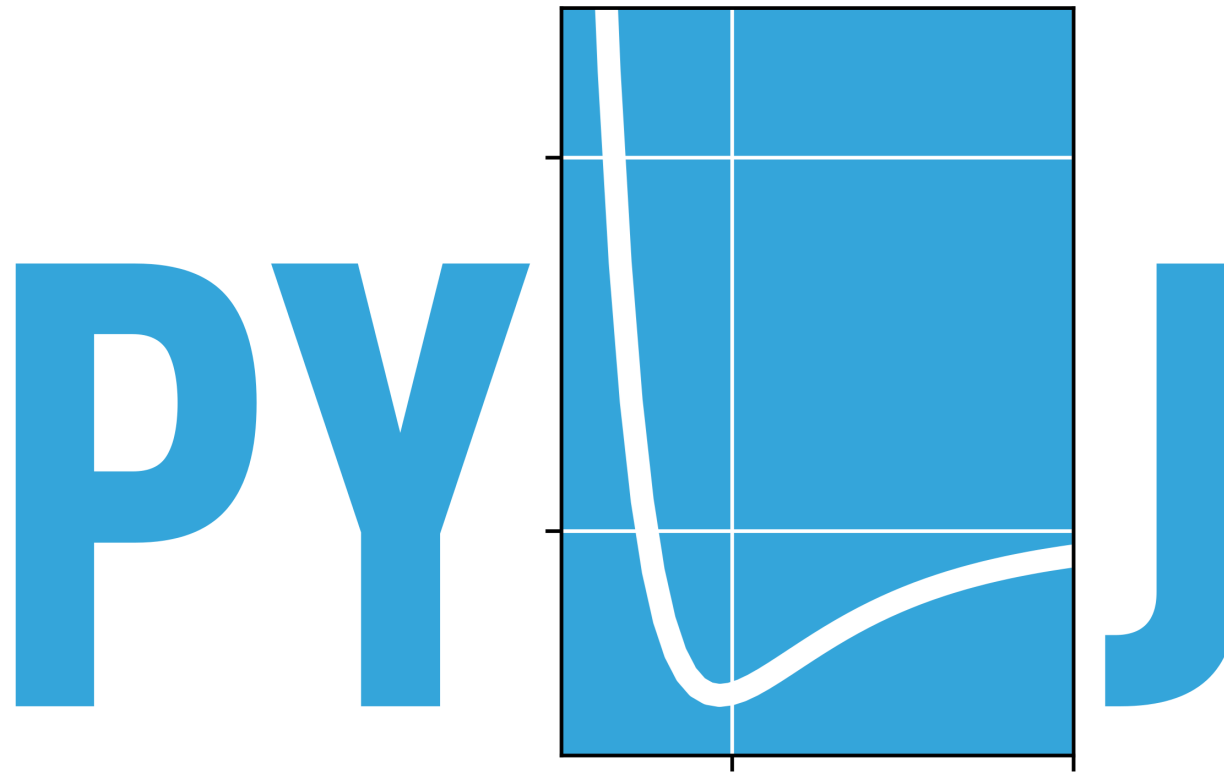
find out more

pythoninchemistry.org/pylj

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Sadie, my dog