Subject: MD/ab initio for polymer solubility?
Posted by muu9 on Mon, 11 Nov 2019 20:26:44 GMT
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I'm an undergraduate doing research in polymer solubility. Is it feasible to take an MD/ab initio/QM approach to estimating the solubility of a large polymer such as Polyethylene? Formula-based methods don't work well due to its unusual (regular) structure.

I've looked here: opensourcemolecularmodeling . github . io/README . html#quantum-chemistry and needless to say I'm a bit out of my depth. Which of these programs are relevant to solubility, and where do they stand in terms of cost/precision trade-off?

My institution also gives me access to the complete Schrodinger suite as well as HSPiP (although the latter's most basic methods don't work too well). Should I use these instead, perhaps with Y-MB method?