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?

Subject: Re: MD/ab initio for polymer solubility?
Posted by nbehrnd on Wed, 13 Nov 2019 20:02:37 GMT
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Right on the spot I would like to suggest to you to deposit this question on Stackexchange Chemistry (https://chemistry.stackexchange.com/) which has a broad spectrum of readers. Because users may gauge their interest to special topics, you may increase the likelyhood of assistance by adding labels relevant to your question (tags), for example «polymers», «computational chemistry», «solubility», «molecular-dynamics». If you may demonstrate briefly what you tried on your own to solve the problem, chances are even higher to find help.

As by today, the abbrevated search for «polymer*» .AND. «solub*» yiels 113 posts (https://chemistry.stackexchange.com/search?q=polymer*+solub*), so try it.

Good luck,
Norwid