Material design using Martini

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Propositions

1. Method development without practical usage information, such as tutorials and examples, only advances one's own science but not the scientific community.
2. A proof-of-concept study is always useful, even if just to inspire other researchers on what to do and what not to do.
3. Software supporting computational research is sometimes undervalued in the molecular simulation community; yet when developed openly and sustainably, it opens the door to access previously impossible research.
4. Titration effects in coarse-grained Martini simulations can be captured semi-quantitively by introducing explicit protons in the model. (Chapter 6)
5. With the highly transferable Martini 3 polymer models, unravelling the true complexity of combinatorial chemistry is within reach of coarse-grained simulations. (Chapter 4 and 5).
6. A self-avoiding random walk can be biased to achieve specific end-to-end distances or even connect onto itself. (Chapter 3)