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Computer-aided Ionic Liquids Design for Separation Processes

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Propositions

Accompanying the thesis

Computer-aided Ionic Liquids Design for Separation Processes

Daili Peng

1. Ionic liquids are promising alternatives to organic solvents despite their relatively high prices.
2. Many computer-aided ionic liquids design (CAILD) results in the literature are arguable because the designed ILs display very complex structures and are hard to be synthesized, making experimental verification cumbersome. (Purif. Technol., 2014, 155, 45-57; Chem. Eng. Sci., 2017, 162, 364-374)
3. The NRTL parameters reported in the literature are sometimes questionable and topological analyses are necessary to test their reliability. (J. Chem. Thermodyn., 2010, 42(4), 484-490)
4. It is better to use multi-objective optimization procedures for CAILD. (Chapter 1 & 4)
5. The toxicity of ILs is often underestimated and should be treated as a constraint when designing IL solvents. (Chapter 2)
6. The limitation of the CAILD method lies in missing parameters for the prediction of physicochemical properties of ILs. (Chapter 3)
7. Due to the recent availability of experimental data, screening methods or algorithms based on big data (e.g. machine learning) are very suitable to select ILs for separation problems. (Chapter 5)
8. Integration of the CAILD method with process design is highly desirable.
9. The thing I have learned from my Ph.D. journey is that you do not have to worry about the outcome, do what is needed.
10. We should always learn from others, by standing on the shoulders of Giants we can see further. (freely adapted from Sir. I. Newton)