Polyethylene oxide force field

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| --- | --- | --- | --- |
| Solvent | Salt | Force field | Paper |
| PEO | |  | | --- | | LiTFSI | | |  | | --- | | TRAPPE-UA | | [*Macromolecules, 2021 (Rui Wang, UC Berkely)*](https://pubs.acs.org/doi/full/10.1021/acs.macromol.0c01850) |
| PEO | |  | | --- | | LiTFSI | | TRAPPE-UA with charge scaling | [*Macromolecules, 2021 (Rui Wang, UC Berkely)*](https://pubs.acs.org/doi/full/10.1021/acs.macromol.1c00995) |
| PEO | LiTFSI | OPLS-AA with charge scaling (0.75) | [*New J. Chem., 2023 (* *Schnell , NTNU)*](https://pubs.rsc.org/en/content/articlepdf/2017/cp/c7cp00526a) |
| PEO | LiTFSI | General Amber Force Field (GAFF) | [*J. Am. Chem. Soc.,2022 (* Chao Zhang, *Uppsala University)*](https://pubs.acs.org/doi/full/10.1021/jacs.2c02389) |
| PEO | LiTFSI | COMPASS | [*Adv. Energy Mater., 2024, (Derrick Wen Hui Fam, Nanyang Technological University)*](https://onlinelibrary.wiley.com/doi/epdf/10.1002/aenm.202402986) |
| PEO | LiTFSI | Scaled charge model | [*J. Chem. Phys. 2015, (Daniel Brandell, Uppsala University)*](https://pubs.aip.org/aip/jcp/article-abstract/143/2/024904/824901/Polymer-ionic-liquid-ternary-systems-for-Li?redirectedFrom=fulltext) |
| Tetraglyme | LiTFSI | TRAPPE-UA (Tetraglyme) + All-atom (LiTFSI) | [*J. Phys. Chem. B, 2023 (Rui Wang, UC Berkely)*](https://pubs.acs.org/doi/full/10.1021/acs.jpcb.2c08029) |
| PEO | LiTFSI | OPLS-AA | [*Phys. Chem. 2024 (Amber Mace**, Uppsala University)*](https://pubs.rsc.org/en/content/articlehtml/2024/cp/d3cp04617f) |
| PEO | LiTFSI | Revised OPLS | [*Polymers****2021****, (Chi-Cheng Chiu, National Cheng Kung University)*](https://www.mdpi.com/2073-4360/13/7/1131) |
| PEO | LiTFSI | OPLS-AA | [*Phys. Chem. 2017, (Dormidontova,* *University of Connecticut)*](https://pubs.rsc.org/en/content/articlepdf/2017/cp/c7cp00526a) |
| PEO | LiTFSI | CHARMM and TraPPE-UA | [*Micromachines****2021****, (Takashi Tokumasu, Tohoku University)*](https://www.mdpi.com/2072-666X/12/9/1012) |
| PEO | LiTFSI | all-atoms PCFF+ | [*Chem. Mater. 2018, (Boris Kozinsky , Harvard)*](https://pubs.acs.org/doi/10.1021/acs.chemmater.8b01955) |