LICHEM 1.1: Recent Improvements and New Capabilities

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1. LICHEM 1.1 Program Package

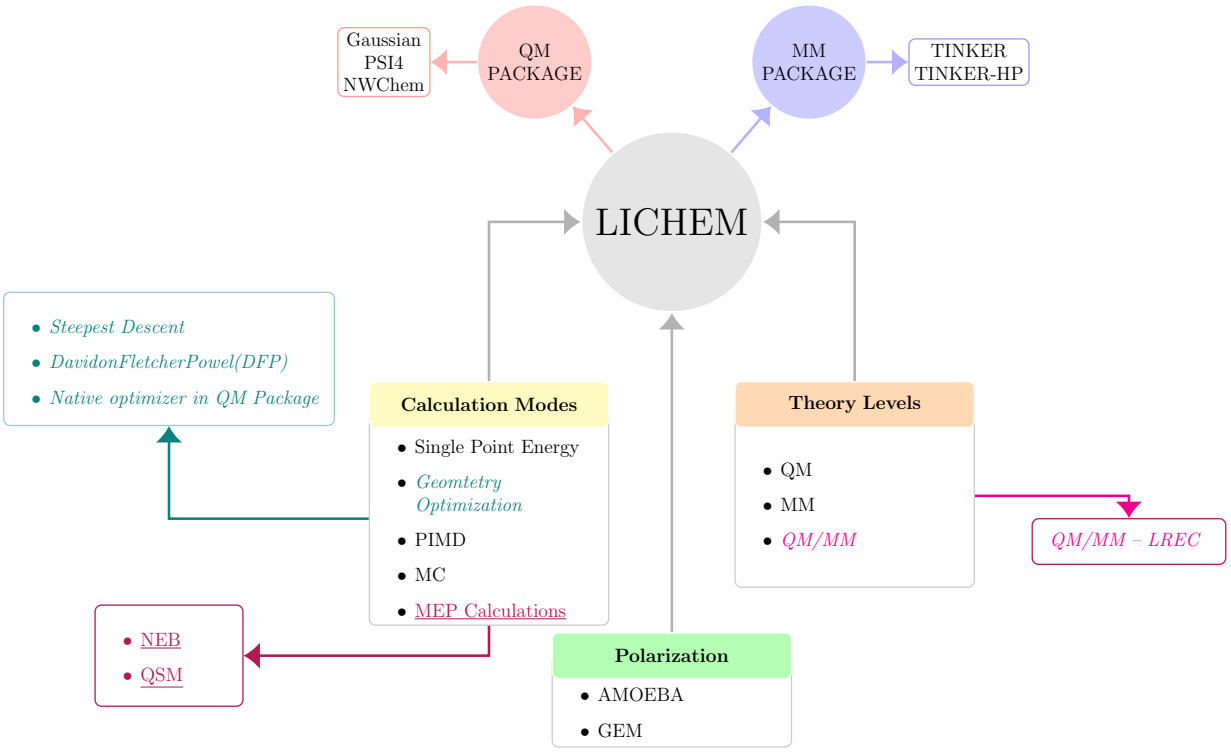

Figure S1: A general flowchart describing the capabilities of LICHEM 1.1 program package for QM/MM simulations.

2. Rate-limiting step in the N-tert-butyloxycarbonylation of aniline in [EMIm][BF_4]

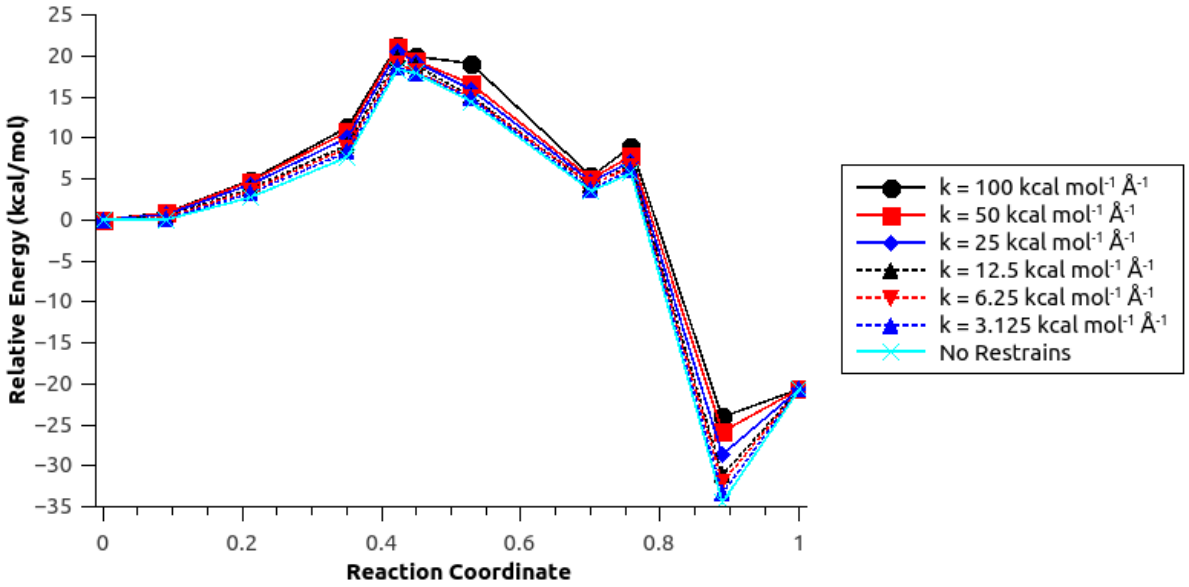

Figure S2: Comparison for the minimum energy path for the aniline nucleophilic attack in each pre-iteration with explicit polarization.

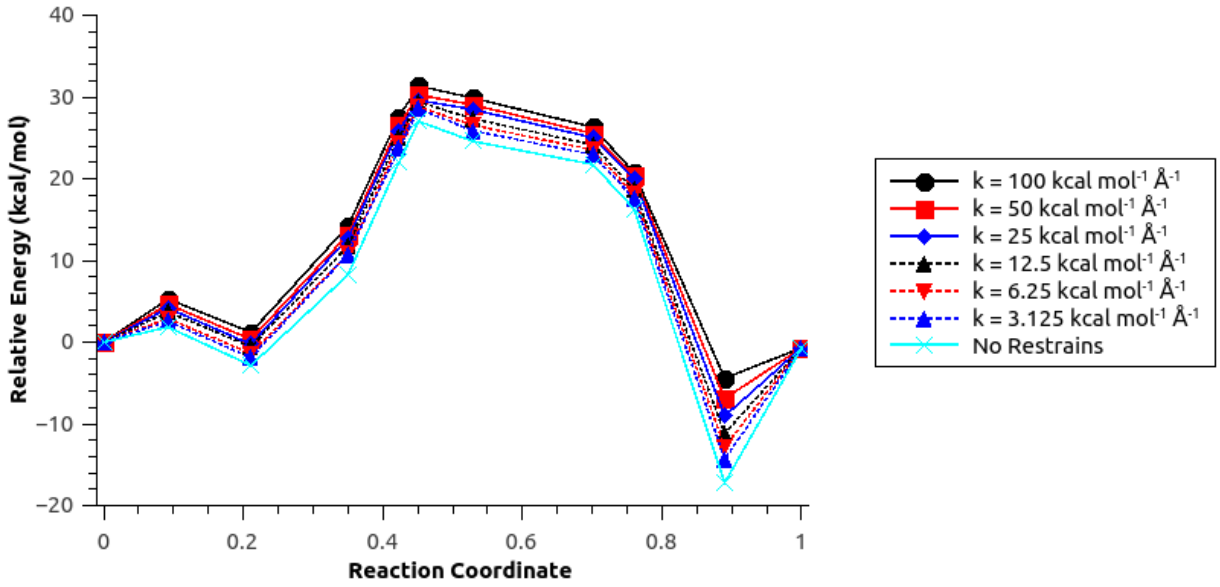

Figure S3: Comparison for the minimum energy path for the aniline nucleophilic attack in each pre-iteration without explicit polarization.

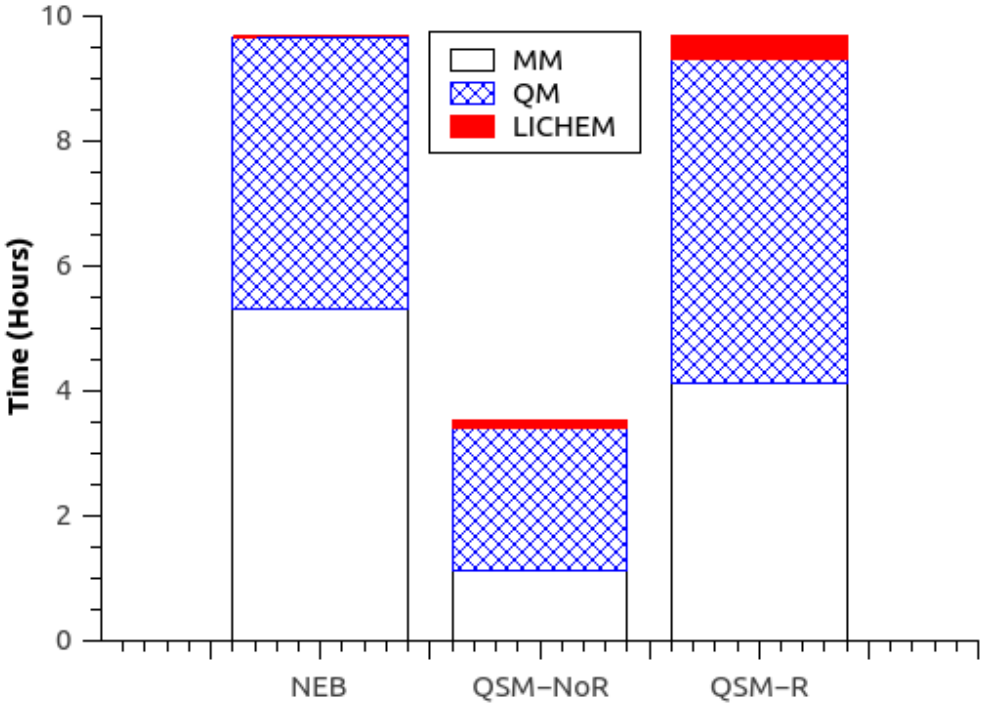

Figure S4: Comparison for the total wall time used in QSM with restrictions (QSM-R), QSM without restrictions (QSM-NoR) and NEB methods with explicit polarization.

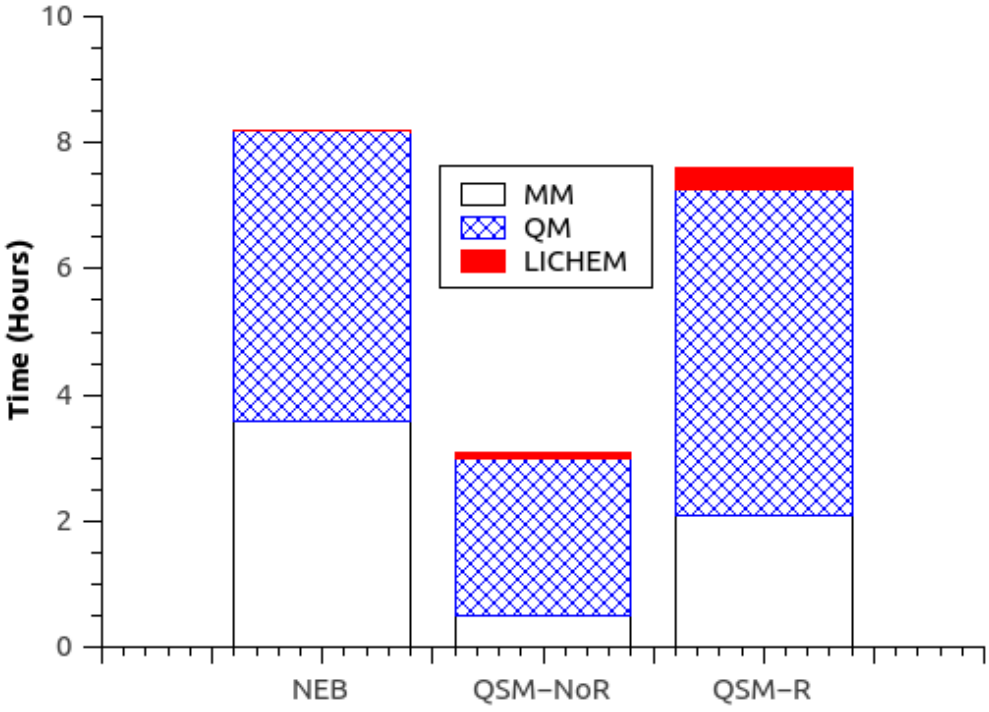

Figure S5: Comparison for the total wall time used in QSM with restrictions (QSM-R), QSM without restrictions (QSM-NoR) and NEB methods without explicit polarization.

3. Example Input for QSM calculations in gas phase for di-Asp System:

QSM Calculations for 9 beads using Gaussian 16 program package[1] at wB97xD level of theory, and TINKER program package[2] with AMOEBA[3] force field. Tolerance for the deviation of the atomic positions in QM region is 1e-2 Å, RMS force tolerance is 0.0025 Hartree/bohr, and maximum force is 0.05 Hartree/bohr. Maximum number of optimization steps is chosen as 10 while maximum number of QSM iteration (QM region) is chosen as 25. Debugging is turned on and all of the outputs are kept with the keywords `debug` and `keep_files` respectively. Frequency is computed for transition state structure (`ts_freq`), and the active atoms are defined by `neb_active` keyword.

Input file:

```
potential_type: qmmm
qm_type: g16
qm_method: wB97xD
qm_basis: GEN
qm_memory: 80 GB
qm_charge: 0
```

qm_spin: 1
mm_type: TINKER
electrostatics: AMOEBA
calculation_type: qsm
beads: 9
nqsm: 0
frozen_ends: yes
qm_opt_tolerance: 1e-2
qm_rms_force_tol: 0.025
qm_max_force_tol: 0.05
mm_opt_tolerance: 1e-1
max_opt_steps: 10
max_qm_steps: 25
pbc: no
keep_files: yes
debug: yes
ts_freq: yes
neb_atoms: 6
14 15 16 39 40 41
qm_atoms: 14
10 11 12 13 14 15 16 35 36 37
38 39 40 41
pseudobond_atoms: 2
8 33
boundary_atoms: 10
6 7 9 17 18 31 32 34 42 43
frozen_atoms: 24
0 1 2 3 4 5 19 20 21 22
23 24 25 26 27 28 29 30 44 45
46 47 48 49

References:

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J., Gaussian 16 Revision A.03. 2016, Gaussian Inc. Wallingford CT
2. Rackers, J. A.; Wang, Z.; Lu, C.; Laury, M. L.; Lagardère, L.; Schnieders, M. J.; Piquemal, J.-P.; Ren, P.; Ponder, J. W. Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273–5289.
3. Ponder, J. W.; Wu, C.; Ren, P.; Pande, V. S.; Chodera, J. D.; Schnieders, M. J.; Haque, I.; Mobley, D. L.; Lambrecht, D. S.; DiStasio, R. A.; Head-Gordon, M.; Clark, G. N. I.; Johnson, M. E.; Head-Gordon, T. Current Status of the AMOEBA Polarizable Force Field. The Journal of Physical Chemistry B 2010, 114, 2549–2564.