Supplementary file: Glossary

Acronym or abbreviation	Meaning
Absorbents	
AA	Amino acid
AEEA	N-(2-aminoethyl) ethanolamine, 2-[(2-Aminoethyl)amino]ethanol
AMP	2-Amino-2-methyl-1-propanol
EDA	ethylenediamine 1,2-Ethanediamine
EG	Ethylene glycol
DEA	Diethanolamine, 2,2'-Iminodiethanol
DEEA	*N*,*N*-Diethylethanolamine
MEA	2-Aminoethanol, ethanolamine, monoethanolamine
MDEA	methyldiethanolamine, 2,2'-(Methylimino)diethanol
MMEA	N-methylethanolamine
PE	2-piperidineethanol
PM	1-Piperidinylmethanol
PZ	Piperazine
TBAE	2-(tert-butylamino)ethanol, 2-[(2-Methyl-2-propanyl)amino]ethanol
TEA	*N*,*N*-Diethylethanamine
TMG	tetramethylguanidine 1,1,3,3-Tetramethylguanidine
TRIS	2-Amino-2-hydroxymethyl-1,3-propanediol
Acronyms	
AIMD	*ab initio* molecular dynamics (non-empirical, first principles quantum mechanics)
ATR	attenuated total reflectance
AUA	anisotropic united-atom force field
BO	Born−Oppenheimer approximation
BSSE	basis set superposition error

CASSCF	complete active space self-consistent field
CBMC	configurational-bias Monte Carlo
CBS	complete basis set extrapolation
CC	coupled clusters theory
GCMC	canonical Monte Carlo
CASSCF	complete active space self-consistent field
CCS	CO_2 capture and storage/sequestration
CCSD	coupled cluster wave functions characterized by iterative inclusion of single and double excitations
CCSD(T)	coupled cluster wave functions characterized by iterative inclusion of single and double excitations with perturbative (4th-order and one term from the fifth order) inclusion of triple excitations
CCSDT	coupled cluster wave functions characterized by iterative inclusion of single, double and triple excitations
CFCMC	continuous fractional component Monte Carlo
CI	configuration interaction
CISDTQ	configuration interaction wave functions incorporated all single and double substitutions as well as triple and quadruple substitutions
CISD[TQ]	configuration interaction wave functions incorporated all single and double substitutions as well as limited triple and quadruple substitutions
CPCM	conductor-like polarizable continuum model
COSMO	conductor-like solvent model
COSMO-RS	conductor-like solvent model for real solvents
COSY	correlation spectroscopy
CSF	configuration state function
CSM	continuum solvation model
DFT	density functional theory
DMC	Diffusion quantum Monte Carlo
EPR	electron paramagnetic resonance
FCI	full configuration interaction
FN-DMC	Fixed-node Diffusion quantum Monte Carlo
FTIR	Fourier transform infrared spectroscopy
GB Method	generalized Born method

GEMC	Gibbs ensemble Monte Carlo
HF	Hartree-Fock
HMBC	heteronuclear multiple-bond correlation spectroscopy
HSQC	heteronuclear single-quantum correlation spectroscopy
IEF-PCM	integral equation formalism-polarizable continuum model
IR	infrared spectroscopy
MC	Monte Carlo
MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
MM	molecular mechanism
MPx	Møller-Plesset perturbation theory (where x is the order of perturbation expansion)
MTC	mass transfer coefficient
NEMD	non-equilibrium Molecular Dynamics simulations
NMR	nuclear magnetic resonance spectroscopy
NPT	isothermal-isobaric ensemble
NVT	canonical ensemble
ONIOM	our own *N*-layered integrated molecular orbital and molecular mechanics
OPLS-AA Force Field	optimized potentials for liquid simulations-all atom force field
OPLS-UA Force Field	optimized potentials for liquid simulations-united atom force field
PBC	periodic boundary condition
PB Equation	Poisson−Boltzmann equation
PCC	post-combustion CO_2 capture
PCM	polarizable continuum model
PES	potential energy surface
QC	Quantum Chemistry
QM	Quantum Mechanics
QMC	quantum Monte Carlo
QM/MM	Quantum mechanics/molecular mechanics (hybrid simulations methods)
QSAR	quantitative structure–activity relationship
ReaxFF	reactive force field
RISM-SCF-SEDD	reference interaction site model–self-consistent field with spatial electron density distribution

RMS	root mean square
RxMC	reaction-ensemble Monte Carlo
SASA	solvent-accessible surface area
SCF	self-consistent field
SCRF	self-consistent reaction-field
SMD	solvent model based on electron density
SMx	solvent model (where x is an alphanumeric label to show the version) which is based on the generalized Born equation
SPC Model	simple point charge model
TraPPE-EH Force Field	transferable potentials for phase equilibria-explicit hydrogen force fields
TraPPE-Pol Force Field	transferable potentials for phase equilibria-polarizable force fields
TraPPE-UA Force Field	transferable potentials for phase equilibria-united atom force fields
TS	transition state
UAHF radii	united atom Hartree–Fock radii
UAKS radii	united-atom Kohn-Sham radii
UFF radii	universal force field radii
UV-vis	Ultraviolet-visible spectrophotometry
VLE	Vapour–liquid equilibrium
VMC	Variational quantum Monte Carlo
μVT	grand canonical ensemble