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A Computational Framework for Evaluating Molecular Dynamics Potential Parameters Employing Quantum Mechanics

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1 Pseudo Code of the Algorithms

Algorithm S1 Nonbonded

```
Start
Create a list of different atom types present in the system
Define the list of different distances value between two atoms as:  [0.05, 1.0] (in steps of 0.05) and
[1.0-3.5] (in steps of 0.5)
for p_i in the list of elements do
   for D_j in the list of distances do
      Set the distance between two atoms equal to D_j
      Set the system's charge based on the atom types
      Run QM simulation to evaluate the total system energy, E_j
      r_j = D_j × √3
      Store the pair of (E_j, r_j)
      Fit the nonbonded force field equation on the (E,D) data
      Save the parameters
   end for
end for
Use mixing rules defined in Equations 2-4 to obtain the potential parameters between dissimilar atom types
Finish
```

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Algorithm S2 Bonded

Start
Create a "Bond-Type" list that contains the different bond types in the molecular system
Create a "Length" list: [-0.6, 0.6] (in steps of 0.05), to vary the bond length
Create a "Bond" list that contains the pairs of atoms for each bond in the system
for $(n_1, n_2)_i$ Bond in "Bond-Type" list do
    Create a "Moving Atoms" list containing all atoms except the group that should be kept fix
    Define a mover vector from atom n_1 to n_2, named $\vec{MV}$
    for C_l in "Length" list. do
        $\vec{MV}_l$ is equal to C_l percent of $\vec{MV}$
        Move all atoms in the "Moving Atoms" list by $\vec{MV}_l$ vector
        Run the QM Simulation to evaluate total system energy (E_l) at Bonded length (l_l)

        Store the pair of (E_l, r_l)
    end for
    Fit an appropriate bonded interaction force field equation to the (E, r) data to evaluate the potential parameters of i^{th} Bond type
end for
Finish

Algorithm S3 Angle

Start
Create the "Angle-Type" list for the different angle types that exist in the system
Define a "Rotation" list containing different rotation angle values in the range [-15, 15]
for $(n_1, n_2, n_3)_i$ in "Angle-Type" list do
    Determine the two leg vectors $\vec{V}_1$ and $\vec{V}_2$
    Calculate the cross product of the leg vectors
    θ_P is the primary angel
    for θ_j in "Rotation" list do
        Rotate the leg vectors about $\vec{V}_r$ based on the θ_j value
        Evaluate new system energy (E_j), employing QM calculations
        Store (E_j, $\theta_j + \theta_P$)
    end for
    Fit an appropriate angle interaction equation to the (E, θ) data
end for
Finish

Algorithm S4 Rotator

Start
Input $\vec{V}$, θ, and $\vec{V}_r$
Create a unite vector from $\vec{V}_r$
Define the rotational matrix $\vec{R} =$ as per Equation **??**
Return $\vec{V}_{new} = \vec{V} \cdot \vec{R}$
Finish

Algorithm S5 Angle Finder

Start
Input the positions of the four atoms (n_1, n_2, n_3, and n_4) participating in the dihedral
Find a plane equation which is perpendicular to the bond between n_2 and n_3
Find the equation of two lines passing n_1 and n_4 and perpendicular to the plane
Find incident points of these lines on the plane
Calculate the angle created by these three points as the Dihedral angle
Finish

Algorithm S6 Dihedral

```
Start
Create a "Dihedral-Type" list containing different dihedral types that exist in the system
Define a "Rotation Angel" list of different rotation angle values in the range [-15, 15]
for (n1, n2, n3, n4)_i in "Dihedral-Type" list do
   Calculate the primarily dihedral's angle (φ_p)
   Define the two leg vectors of the dihedral
   Define the normal vector of the plane perpendicular to the bond between n2 and n3
   for φ_j in "Rotation Angel" list do
      Rotate the leg vectors equal to φ_j
      Evaluate new system energy (E_j), employing QM calculations
      Store (E_j, φ_j + φ_P)
   end for
   Fit and appropriate Dihedral interaction equation to the (E, φ) data
end for
Finish
```

Algorithm S7 Improper

```
Start
Create the "Improper-Type" list containing the different improper types that exist in the system
Define the "Rotation Angle" list containing the different rotation angle values in the range [-15, 15]
for (n1, n2, n3, n4)_i in "Improper-Type" list do
   Find the two planes containing n1, n2, n3 and n2, n3, n4
   Find the primarily improper angle as χ_P
   for χ_j in "Rotation Angel" list do
      Rotate the two planes equal to χ_j
      Evaluate new system energy (E_j), employing QM calculations
      Store (E_j, χ_j + χ_P)
   end for
   Fit an appropriate Improper interaction force field equation to the (E, χ) data
end for
Finish
```

2 Potential Energy Figures

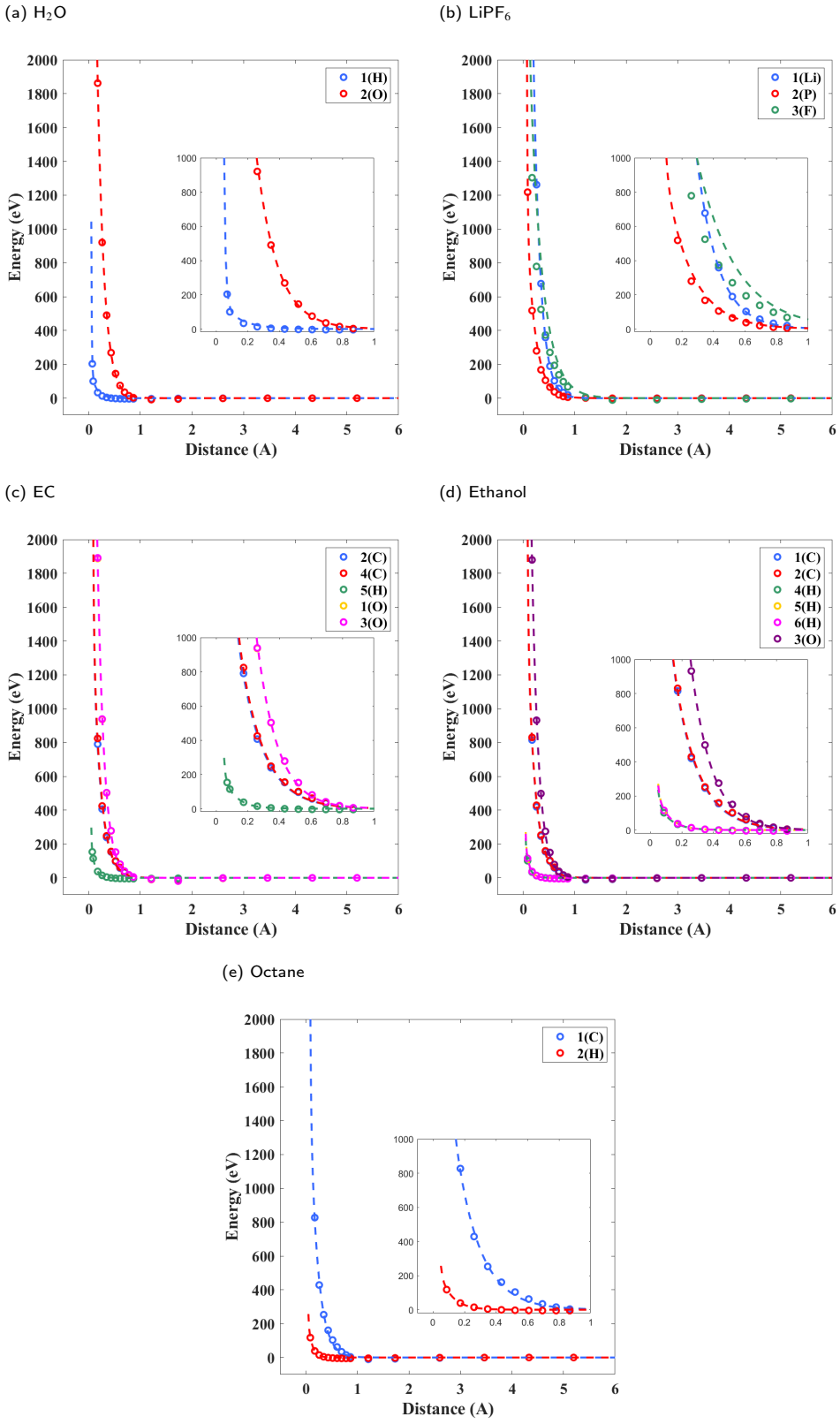

Fig. S1 Data of nonbonded interactions energy as a function of the distance between two atoms of each type using a combination of our algorithms and QM calculation (indicated by symbols). The Buckingham potential equation ($E = Aexp(-\frac{r}{B}) - \frac{C}{r^6}$)) (indicated by the dashed lines) has been fitted to this data.

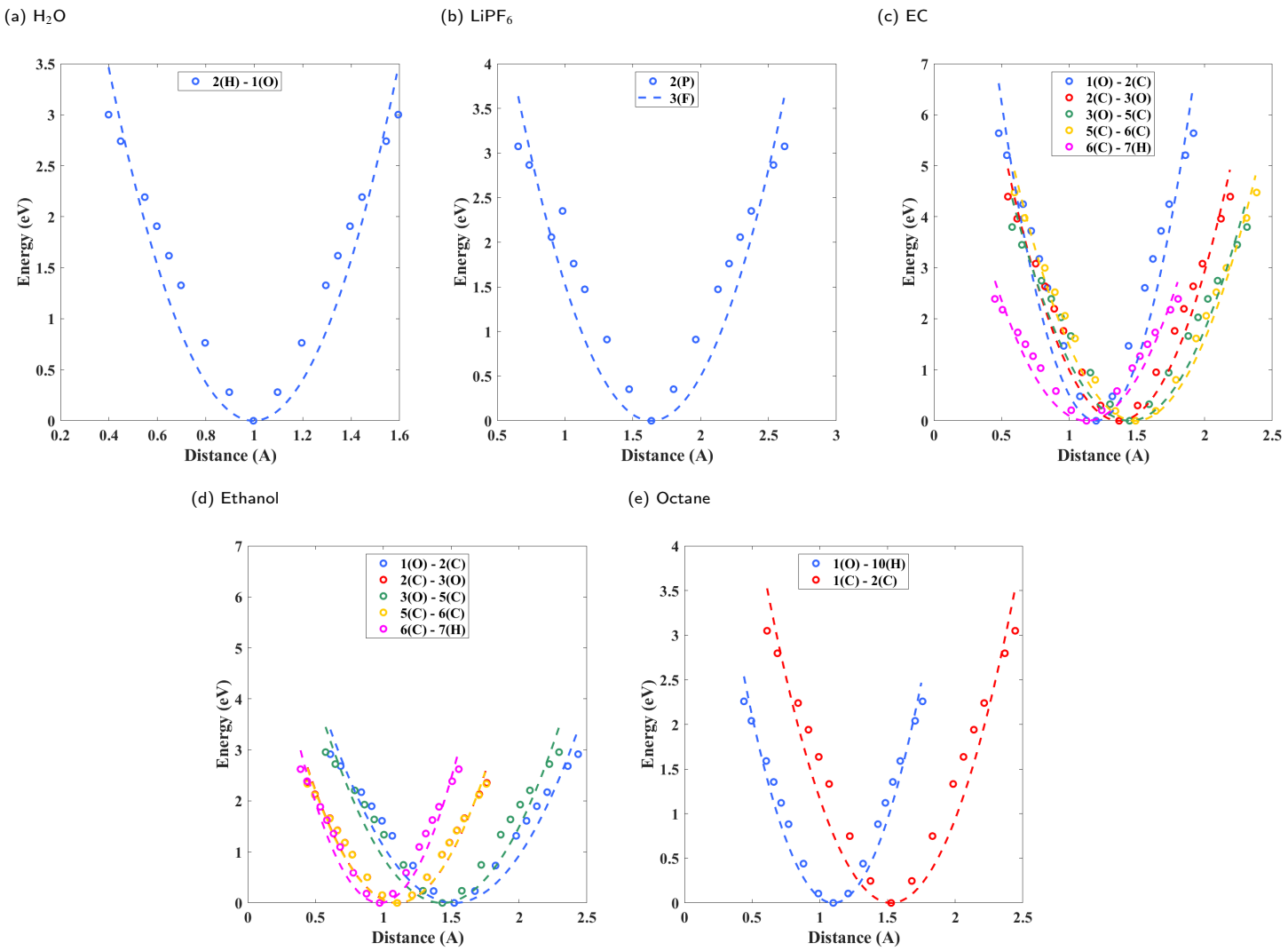

Fig. S2 Estimated bonded interaction energy as a function of the bond length for different bond types in the three molecules. The Harmonic Bonded interaction equation (Table 2) has been fitted on the obtained data points.

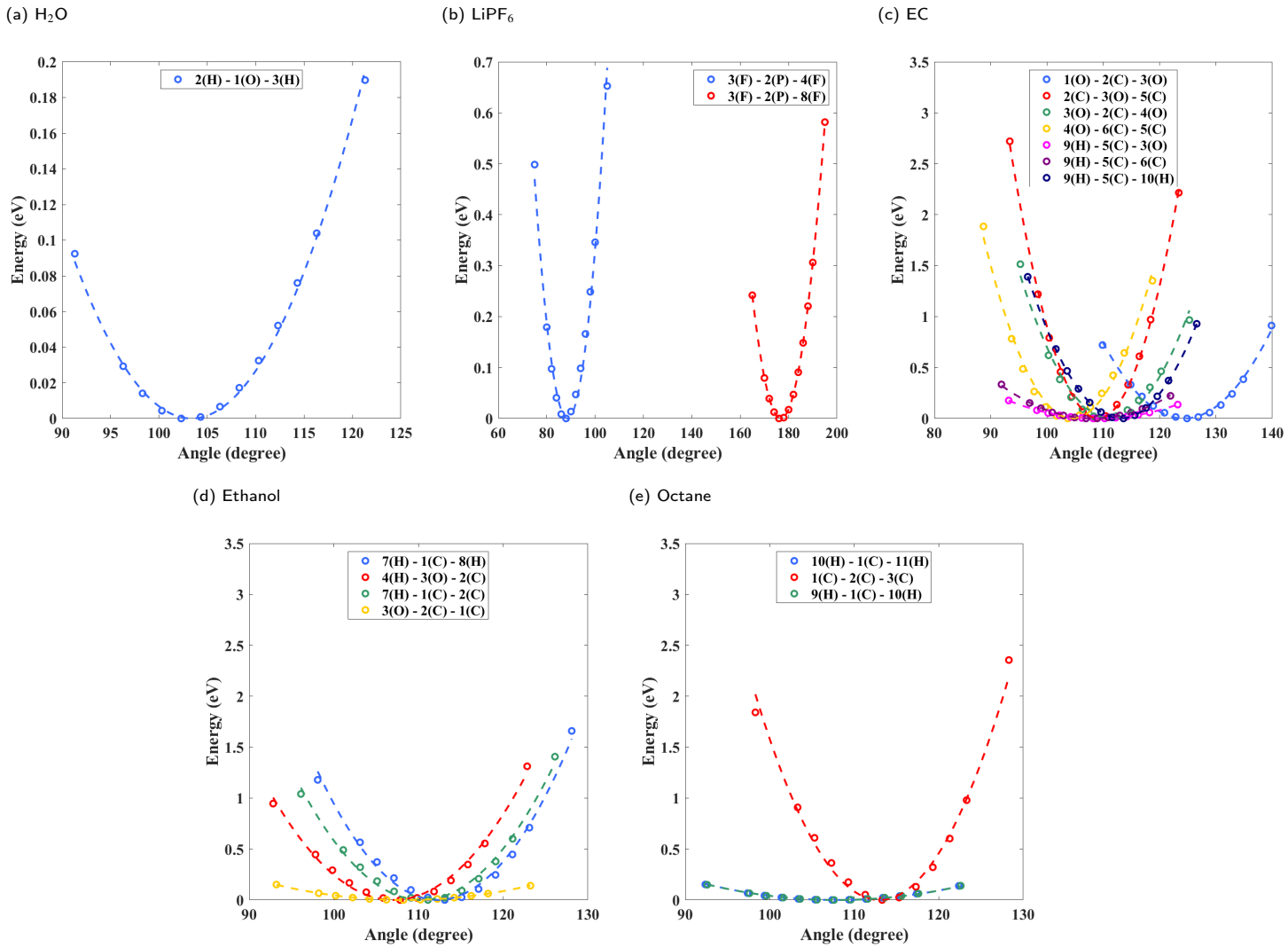

Fig. S3 The data points for the *angle* interaction energy as a function of θ, for the studied molecules, using a combination of Algorithms 3, 4 and QM calculation. The Harmonic Angle style equation (Table 2) is fitted on these data points.

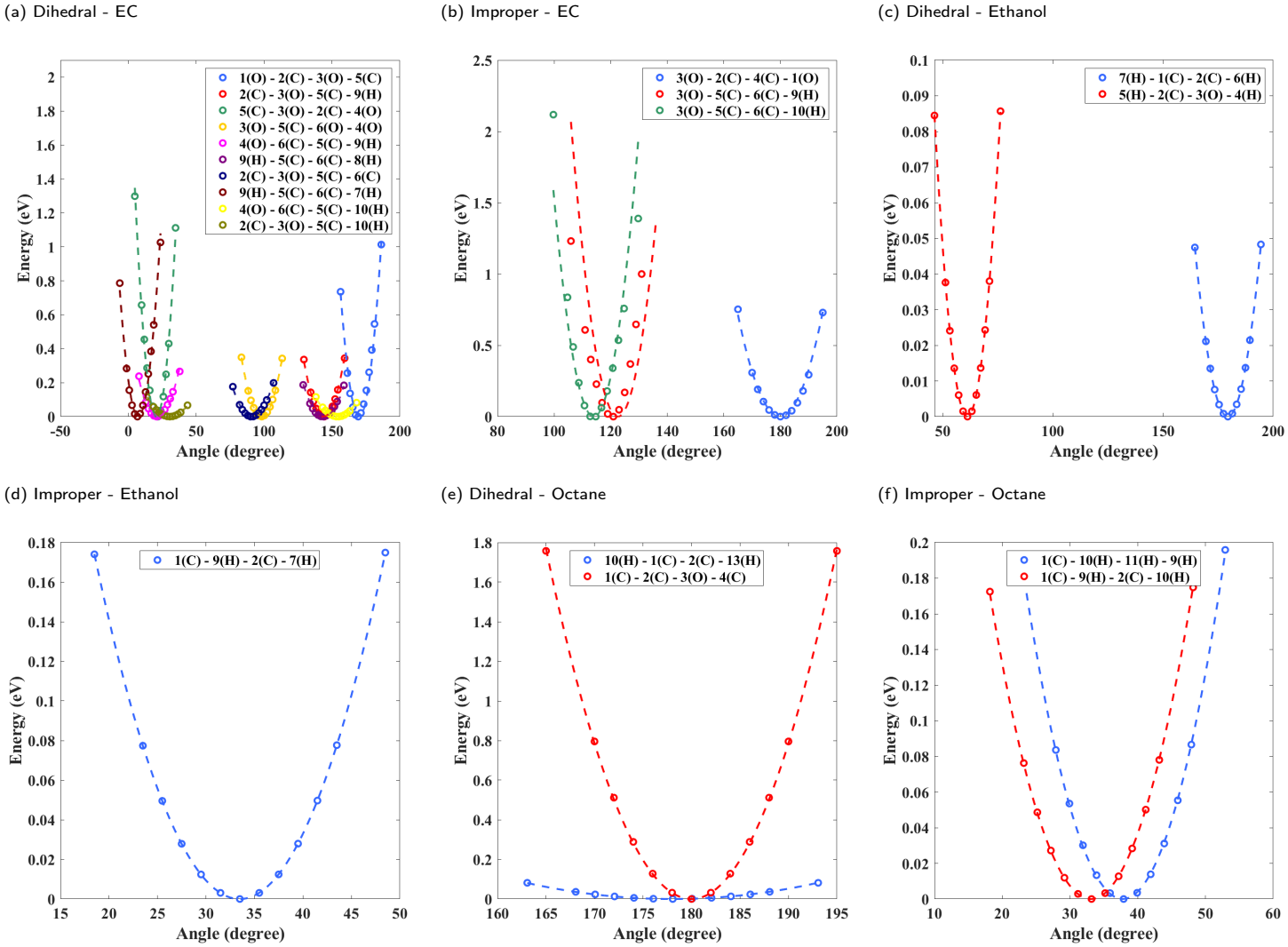

Fig. S4 The data points for the *dihedral* and *improper* interaction energy as a function of ϕ and χ, for EC and Ethanol molecules, have been obtained by employing our algorithms in conjunction with the QM calculation. The Quadric and Harmonic Dihedral and Improper style equations (Table 2), are fitted on these data points.

3 Potential Parameters Values

Type	A	B(Å)	C(Å^6)	R^2
H_2O				
1(O) - 1(O)	$5.65E+3$	$1.43E-1$	$-5.50E-3$	0.99
2(H) - 2(H)	$1.81E+2$	$1.12E-1$	$-1.39E-5$	0.99
$LiPF_6$				
1(Li) - 1(Li)	$1.67E+3$	$1.71E-1$	$-8.72E-2$	0.99
2(P) - 2(P)	$1.71E+3$	$3.21E-1$	$-1.97E-6$	0.99
3(F) - 3(F)	$4.82E+3$	$1.58E-1$	$-7.25E-6$	0.99
EC				
1(O) - 1(O)	$3.37E+4$	$1.12E-1$	$3.59E+0$	0.99
2(C) - 2(C)	$4.37E+3$	$1.47E-1$	$0.46E+0$	0.99
3(O) - 3(O)	$3.66E+4$	$1.11E-1$	$3.88E+0$	0.99
4(C) - 4(C)	$6.93E+3$	$1.33E-1$	$7.66E-1$	0.99
5(H) - 5(H)	$3.89E+2$	$7.56E-2$	$1.61E-6$	0.99
Ethanol				
1(C) - 1(C)	$2.49E+3$	$1.56E-1$	$-3.09E-4$	0.99
2(C) - 2(C)	$2.50E+3$	$1.53E-1$	$-2.99E-4$	0.99
3(O) - 3(O)	$6.85E+3$	$1.35E-1$	$-5.49E-4$	0.99
4(H) - 4(H)	$1.96E+2$	$1.44E-1$	$-2.01E-5$	0.99
5(H) - 5(H)	$3.06E+2$	$8.87E-2$	$-4.97E-6$	0.98
6(H) - 6(H)	$3.00E+2$	$8.99E-2$	$-5.47E-6$	0.98
Octane				
1(C) - 1(C)	$7.95E+3$	$1.31E-1$	$8.58E-1$	0.99
2(H) - 2(H)	$3.55E+2$	$8.01E-2$	$2.03E-6$	0.99

Table S1 Nonbonded potential parameters for the Buckingham potential equation ($E = Aexp(-\frac{r}{B}) - \frac{C}{r^6}$), using the suite of algorithms for the studied molecules.

Type	K ($\frac{eV}{}$)	r_0()	R^2
H_2O			
1(O) - 2(H)	$+9.7002E+0$	$+9.9642E-1$	0.86
$LiPF_6$			
2(P) - 3(F)	$+3.7769E+0$	$+1.6359E+0$	0.78
EC			
1(O) - 2(C)	$+1.2795E+1$	$+1.1988E+0$	0.84
2(C) - 3(O)	$+7.3383E+0$	$+1.3684E+0$	0.92
3(O) - 5(C)	$+5.7992E+0$	$+1.4457E+0$	0.87
5(C) - 6(C)	$+5.9967E+0$	$+1.1275E+0$	0.88
6(C) - 7(H)	$+6.1310E+0$	$+1.4903E+0$	0.96
Ethanol			
1(C) - 7(H)	$+6.0882E+1$	$+1.1012E+0$	0.92
2(C) - 5(H)	$+6.0685E+0$	$+1.0994E+0$	0.92
1(C) - 2(C)	$+4.0770E+0$	$+1.5220E+0$	0.86
2(C) - 3(O)	$+4.6610E+0$	$+1.4342E+0$	0.85
3(O) - 4(H)	$+8.7982E+0$	$+9.7215E-1$	0.90
Octane			
1(C) - 2(C)	$+4.1993E+1$	$+1.5271E+0$	0.87
1(C) - 9(H)	$+5.8337E+0$	$+1.0996E+0$	0.93

Table S2 Bonded potential parameters for the Harmonic style equation ($E = K(r - r_0)^2$) for the five molecules.

Type	K ($\frac{eV}{rad}$)	θ_0(deg)	R^2
H_2O			
2(H) - 1(O) - 3(H)	$+1.9910E+0$	$+1.0336E+2$	0.99
$LiPF_6$			
3(F) - 2(P) - 4(F)	$+8.3750E+0$	$+8.8599E+1$	0.99
3(F) - 2(P) - 8(F)	$+5.7379E+0$	$+1.7677E+2$	0.99
EC			
1(O) - 2(C) - 3(O)	$+1.1835E+1$	$+1.2433E+2$	0.99
2(C) - 3(O) - 5(C)	$+3.5900E+1$	$+1.0908E+2$	0.99
3(O) - 2(C) - 4(O)	$+1.7875E+1$	$+1.1132E+2$	0.98
4(O) - 6(C) - 5(C)	$+2.3454E+1$	$+1.0451E+2$	0.99
9(H) - 5(C) - 3(O)	$+2.2683E+0$	$+1.0910E+2$	0.99
9(H) - 5(C) - 6(C)	$+3.9920E+0$	$+1.0823E+2$	0.99
9(H) - 5(C) - 10(H)	$+1.6783E+1$	$+1.1310E+2$	0.99
Ethanol			
7(H) - 1(C) - 8(H)	$+2.1289E+1$	$+1.0840E+2$	0.99
4(H) - 3(O) - 2(C)	$+1.6393E+1$	$+1.0702E+2$	0.99
7(H) - 1(C) - 2(C)	$+1.7807E+1$	$+1.1036E+2$	0.98
3(O) - 2(C) - 1(C)	$+2.0673E+0$	$+1.1225E+2$	0.99
Octane			
1(C) - 2(C) - 3(C)	$+3.0673E+1$	$+1.1283E+2$	0.99
10(H) - 1(C) - 11(H)	$+2.1239E+0$	$+1.0764E+2$	0.99
9(H) - 1(C) - 10(H)	$+2.1117E+0$	$+1.0777E+2$	0.99

Table S3 Angle potential parameters for the Harmonic style equation ($E = K(\theta - \theta_0)^2$) for the five molecules.

EC			
Dihedral			
Type	K ($\frac{eV}{rad}$)	ϕ_0(deg)	R^2
1(O)-2(C)-3(O)-5(C)	$+1.268E+1$	$+1.696E+2$	0.99
2(C)-3(O)-5(C)-9(H)	$+5.047E+0$	$+9.830E+1$	0.99
5(C)-3(O)-2(C)-4(O)	$+1.317E+1$	$+7.270E+0$	0.99
3(O)-5(C)-6(O)-4(O)	$+3.690E+0$	$+2.168E+1$	0.99
4(O)-6(C)-5(C)-9(H)	$+2.729E+0$	$+9.116E+1$	0.99
9(H)-5(C)-6(C)-8(H)	$+1.312E+0$	$+3.060E+1$	0.99
2(C)-3(O)-5(C)-6(C)	$+1.758E+1$	$+2.062E+1$	0.99
9(H)-5(C)-6(C)-7(H)	$+1.433E+0$	$+1.543E+2$	0.99
4(O)-6(C)-5(C)-10(H)	$+2.700E+0$	$+1.435E+2$	0.99
2(C)-3(O)-5(C)-10(H)	$+4.958E+0$	$+1.441E+2$	0.99
Improper			
Type	K ($\frac{eV}{rad}$)	χ_0(deg)	R^2
2(C)-3(O)-4(C)-1(O)	$+2.509E+0$	$-2.383E-1$	0.99
3(O)-2(C)-4(C)-1(O)	$+1.057E+1$	$+1.798E+2$	0.99
5(C)-3(O)-6(C)-9(H)	$+3.068E+0$	$+3.299E+1$	0.99
Ethanol			
Dihedral			
Type	K ($\frac{eV}{rad}$)	ϕ_0(deg)	R^2
7(H)-1(C)-2(C)-6(H)	$+1.241E0$	$+6.110E+1$	0.99
5(H)-2(C)-3(O)-4(H)	$+6.985E-1$	$+1.793E+2$	0.99
Improper			
Type	K ($\frac{eV}{rad}$)	χ_0(deg)	R^2
1(C)-9(H)-2(C)-7(H)	$+2.545E+0$	$+3.348E+1$	1.00
Octane			
Dihedral			
Type	K ($\frac{eV}{rad}$)	ϕ_0(deg)	R^2
1(C)-2(C)-3(C)-4(C)	$+2.577E1$	$+1.800E+2$	1.0
10(H)-1(C)-2(C)-13(H)	$+1.192E0$	$+1.780E+2$	1.0
Improper			
Type	K ($\frac{eV}{rad}$)	χ_0(deg)	R^2
1(C)-10(H)-11(H)-9(H)	$+2.793E+0$	$+3.779E+1$	1.00
1(C)-9(H)-2(C)-10(H)	$+2.533E+0$	$+3.313E+1$	1.00

Table S4 Dihedral and Improper potential parameters of EC, Ethanol and Octane molecules for Quadratic and Harmonic potential style ($E = K(\phi - \phi_0)^2$, $E = K(\chi - \chi_0)^2$).