Introducing a novel method based on ICA algorithm to determination of fluorine intermolecular potential from ab initio calculations

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Introduction

We propose new procedure by which one of the newest meta-heuristic algorithms which called Imperialistic Competitive Algorithm (ICA) [1] is used to find the best functional form and the best set of parameters to fit the energies provided by ab initio calculations.

Computational and Methodology

The basis set superposition error corrected potential energy surface of F_2-F_2 system is calculated at CCSD(T) level of theory. Interaction energies obtained using the aug-cc-pVDZ and aug-cc-pVTZ basis sets are extrapolated to the complete basis set limit (CBS) using the newest extrapolated scheme [2]. Calculations are performed for 44 different orientations and 1320 points of F_2–F_2 system. In this work, attempts have been applied to assign a higher weight to the points in the attractive region. An appropriate objective function for the system is defined as:

$$F = \frac{\sum_{i=1}^{N_a} |E_{ICA}(r) - E_{abi}(r)| e^{-\gamma_i}}{N_a} + \frac{\sum_{j=1}^{N_r} |E_{ICA}(r) - E_{abi}(r)| e^{-\gamma_j}}{N_r} \quad (1)$$

The first part of objective function is related to attraction points and the second part is related to repulsive points. Here, E_{ICA} is the energy obtained by ICA algorithm, E_{ab} is the energy obtained using ab initio calculation, γ is the normalized energy, N_a and N_r are the numbers of attractive and repulsive points, respectively.

Results and discussion

The potential parameters obtained from the ICA algorithm of the Lennard-Jonse (LJ) potentials are reported in Table1.

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Table1: The potential parameters for the potential model LJ obtained in this work.

Potential form	Potential parameters	
LJ	$\varepsilon\ (cm^{-1})$	89.12
	$\sigma\ (\text{Å})$	3.11

The value of $B_2(T)$ for a given temperature T is calculated from the following equation:

$$B_2(T) = -2\pi N_A \int_0^{\infty} \exp\left(\frac{-U(R)}{kT} - 1\right) R^2 dR \qquad (2)$$

where k and N_A are Boltzmann and Avogadro constants, respectively. The second virial coefficients calculated using LJ potential obtained from the ICA algorithm are compared with experimental data in Table 2.

Table 2. Temperature dependence of the second virial coefficient $B_2(T)$ ($cm^3\ mol^{-1}$) (experimental and calculated values)

T(K)	115	120	125	130	135	140	145	150
$B_2(T)$/Ref. [3]	-130.1	119.4	110	-101.7	-94.2	-87.5	-81.5	-75.9
This work	-127.98	-118.40	-109.9	-102.31	-95.49	-89.33	-83.75	-78.66

Conclusion

Values of the second virial coefficient, as calculated by the Lennard-Jonse potential and ICA algorithm, provide a good description of the available experimental data. This agreement indicates that the use of such model is appropriate and does not limit the accuracy of simulations.

References

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