**Introduction**

The lithium chemistry has received a great attention in recent years due to the importance that LiH molecules and its ionic variants can have in the primordial universe [1,2]. The reaction LiH + H → Li + H₂ is considered to contribute to LiH depletion, while the hydrogen-exchange reaction LiH + H → LiH + H leads to the retention of LiH in this process.

In this work we report our recent studies on the long-range interactions between the reactants of those reactions. For the LiHH system, the main contribution for the long-range interactions is the dispersion interaction. To modeling the dispersion interaction, the parallel and perpendicular values of the polarizabilities, α, for the diatomics (H-H and Li-H) have been calculated and fitted using the follow equation (see figure).

\[ F(R) = A + \sum_{\alpha, \beta} B_{\alpha, \beta} R^{\alpha+3} + C_{\alpha, \beta} R^{\alpha+1} (1 - \exp(-R^2)) \]

\[ + (1 - \exp(-R^2))^2 E_0/R^6 + (1 - \exp(-R^2)) E_0/R^6 \]

\[ \alpha \quad \beta \]

**Dispersion interaction coefficients**

The dispersion interaction coefficients Cₙ can then be computed as C₈ and C₁₀ have been semiempirically estimated from C₆ using a universal correlation.

\[ N_{\text{eff}} (R) = N_{\infty} + [a + b(R - R_0)] \exp[c(R - R_0)] \]

We found it convenient to use the follow expression for the variation of Neff with the diatomic distance.

The parameters a, b and c have been defined in order to reproduce the united atom and far apart, Neff limits as well as an equilibrium value, if known.

To better model the dispersion interaction we need the coefficients Cₙ(AB - C) (R), n = 8 and 10. When available we have used literature values, otherwise, we have semiempirically estimated those coefficients from C₈ using a universal correlation.

\[ C_n^{1,1}(AB - C) (R) = C_6^{1,1}(AB - C) (R) \exp \left( \frac{R_0(n+6)^n}{(AB - C) (R)} \right) \]

In lack of accurate values for the Le Roy's parameter, R₀(AB - C)/R₀, we have estimated it using the follow equation, where we use the mean polarizability of the diatomic as a measure of the diatomic volume and the atomic radius is taken from the literature.

\[ R_0(AB - C) (R) = 2 \left[ \sqrt{\alpha_{AB}(0)} (R) \right]^{\frac{1}{2}} + \left[ \sqrt{\alpha_{C}(0)} \right]^{\frac{1}{2}} \]

The total dispersion interaction will be computed as a function of Cₙ and inter-atomic distances [3].

\[ C_n(R_i, \theta_i) = \frac{1}{3} \left( 2 C_n^1(R) + C_n^0(R) \right) + \frac{1}{3} \left( C_n^1(R) - C_n^1(R) \right) \]

\[ \times 3 \cos^2 \theta_i - 1 \]

The dynamical correlation energy has been computed using the follow equation.

\[ V_C = \sum_{i=1}^{3} S(R_i, \theta_i) \sum_{i=1}^{10} C_n^0(R_i, \theta_i) \chi_n(r_i) \]

\[ + \sum_{i=1}^{3} \sum_{j>i}^{3} \left[ 1 - S(R_{ij}, \theta_{ij}) \right] \sum_{i=1}^{10} C_n^0(R_i, \theta_i) \chi_n(r_{ij}) \]

The dynamical correlation energy is shown for the interaction Li-HH and H-LiH, at different approaching angles between atom and diatomic molecule 0°, 45° and 90°.

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**References:**