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Fitting Potential Energy Curves (PEC) For Diatomic Molecules.

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Fitting potential energy curves (PEC) for diatomic molecules becomes a well-established routine confirmed empirically with numerous examples in the literature. One of the questions, which remains still open concerns the extrapolation properties of the potential functions. The experimental PECs virtually always are determined from a limited set of experimental data and this in turns limits the range of internuclear distances where the shape of the potential is unambiguously fixed. Extrapolations are usually unreliable because there is no universal analytic form which parametrizes all possible potentials. Exception is the long-range form of the potential, where the inverse-power expansion De-Cn/Rn- Cm/Rm-... is valid with powers n, m etc., which depend on the atomic asymptote.

The Morse-Long-Range (MLR) potential (Mol. Phys. 105, 663 (2007)) has been reported to have a built in long-range asymptotic behavior and therefore it is plausible to expect that one can expect good extrapolation properties and even possibility to determine important molecular parameters like De or/and Cn from limited set of experimental data.

In this contribution we will study the extrapolation properties of the MLR potential and the uncertainty of De and Cn. The studies will be based on Monte-Carlo approach and will be based on real experimental data.

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