Potential Formulation for CNT

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INTRODUCTION

The precise description of interatomic interactions within and between carbon nanotubes and other molecules/atoms requires a potential function dependent on the interatomic distance. This work delves into constructing such a function, specifically considering the unique geometrical characteristics of CNTs.

PROCEDURE

1. Characterize the two types of rings and observe the intrinsic symmetries.
2. Formulating the Lenard-Jones Potential for CNT-H interaction.
3. Two cases have been studied, considering the symmetries - the first considering the particle going through the closely spaced rings, and the second considering the particle going through the relatively far-apart rings.
4. Successively add rings and check for changes to the potential function.
5. Fixing a certain level of accuracy for the system and formulating the potential function.

DATA

RING TYPE	X COORDINATES	Y COORDINATES
Ring A	1.957218, -1.583422, 0.604813, -1.583422, 0.604813	0.0000, 1.150424, -1.861425, -1.150424, 1.861425
Ring B	1.583422, -0.604813, 1.583422, -1.957218, -0.604813	-1.150424, -1.861425, 1.150424, 0.0000, 1.861425

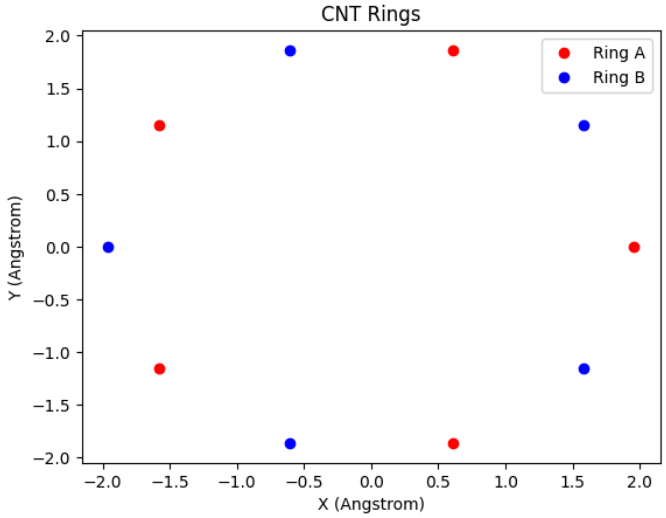

Figure 1. Positions of C atoms in the two types of rings

RESULTS

It was found computationally that 40 rings describe the potential reasonably accurately. Hence, the final potential function was calculated by approximating the number of rings considered for potential calculation as 40. The potential plots were obtained as given in Figure 2 and Figure 3.

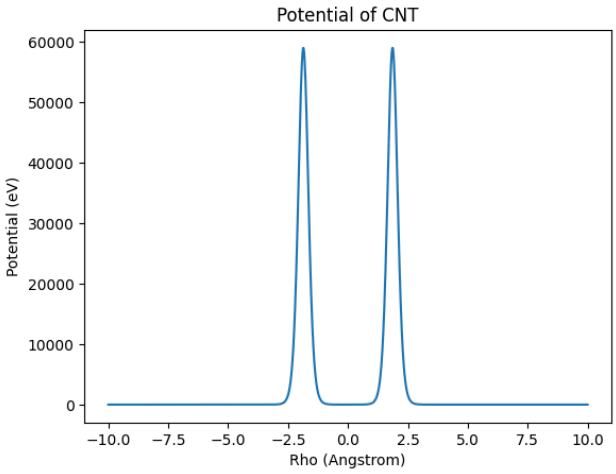

Figure 2. Potential for Case 1.

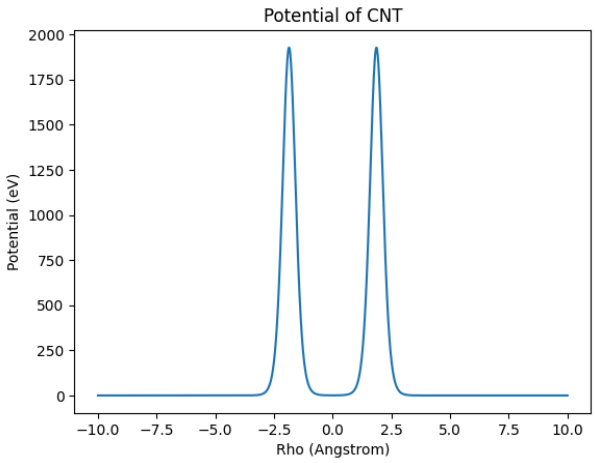

Figure 3. Potential for Case 2.

CONCLUSION

The potential function was constructed for CNT - H atom interaction.

REFERENCES

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