

Review of the article entitled

A Modulation Method of Endohedral Fullerene Material: Using the external electric field, by Qianjin Xiang, Yuzhu Liu, Yu Chen, and Jinyou Long

This article is within the scope and suitable for publication in the journal Chemical Physics Letters after some revision.

The English language should be improved at some places.

In the abstract, state In recent years, once at the beginning of the sentence, without repeating after endohedral fullerene materials

In Highlights, N@C₆₀ was taken as an example, instead of was taken an example

Use C₆₀ with the subscript in the entire manuscript, instead of C60 at some places

Use singular for endohedral fullerene N@C₆₀ in ground state, instead of endohedral fullerenes N@C₆₀ in ground states, as well as for C₆₀ in ground state, in the legends of Figures, captions of Tables and in the entire manuscript

Use one space between the number and the adequate unit of measure, for example on page 2 of the manuscript, 1 a.u.,
on page 4, 27.2114 eV
on page 7, 2.7 eV

Place the adequate number and unite of measure in the same row in the entire manuscript, for example on page 6, 0.01 a.u. and -0.23063 a.u.

On page 4, the second sentence should be
The higher the power of the EEF, the greater the effect on the total energy.

Use small first letters for both alpha molecular orbitals (MOs) and beta MOs, instead of Beta MOs

On page 7,
It is obvious than the effect of the EEF on beta MOs is greater than on alpha MOs.
have the same behavior, instead of a same behavior
In the first sentence of the second paragraph, the LUMO energy and HOMO energy of alpha MOs and beta MOs are shown in Fig. 3 and Fig. 4, respectively
In the second sentence, due to the closeness of their energy

On page 8, the frequencies of absorption peaks of IR spectrum of N@C₆₀ in ground state are consistent with the frequencies of absorption peaks of C₆₀ in ground state

On page 9, state the same correct value of 504.16 cm⁻¹, both in Table 2 and in the text

According to the calculated results, instead of According the calculated results

On page 10, use plural for Two absorption peaks at the frequencies of 1112.09 cm^{-1} and 1232.57 cm^{-1} , and the detailed parameters of the strongest vibrational modes of them
Mention the same correct value of 1112.09 cm^{-1} in the next sentence
the infrared intensity of vibrational mode at a frequency of 1232.57 cm^{-1} increases from 0 a.u. to 5.152 a.u., instead of increase

Specify the unit of measure after the number, 15.0952 a.u.

Use plural or singular at the adequate places in the entire sentence

The Raman spectra of endohedral fullerenes $\text{N}@C_{60}$ are studied with DFT at B3LYP/3-21G level.

The Raman spectrum of endohedral fullerene $\text{N}@C_{60}$ in ground state is obtained.

On page 11, the calculated result of Raman spectrum of $\text{N}@C_{60}$ in ground state is close to that of C_{60}

On page 12, the strongest vibration mode of the Raman spectrum of endohedral fullerene $\text{N}@C_{60}$, is affected by the EEF greatly

Put points at the end of the legend of the figures and format the entire manuscript, including all references according to the style of the journal.

Add the last page numbers to references 3, 5, 12 and 28

The names of the journals in references 5 and 21 should be italic

In reference 21, the number of volume should be placed before the year (2018)

Reviewer comments submitted to the website of the journal Chemical Physics Letters.

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