|  |
| --- |
|  |
| Book Name: | [**Chemical and Materials Sciences: Research Findings**](https://www.bookpi.org/bookstore/product/chemical-and-materials-sciences-research-findings-vol-1/) |
| Manuscript Number: | **Ms\_BPR\_4945** |
| Title of the Manuscript:  | **Unusual chemical bond and spectrum of beryllium dimer in ground X1Σ+g state** |
| Type of the Article | **Book Chapter** |

**Special note:**

**A research paper already published in a journal can be published as a Book Chapter in an expanded form with proper copyright approval.**

**Source Article:**

**This chapter is an extended version of the article published by the same author(s) in the following journal.**

**Journal of Quantitative Spectroscopy and Radiative Transfer, 262, March 2021, 107529.**

**Available:** [**https://doi.org/10.1016/j.jqsrt.2021.107529**](https://doi.org/10.1016/j.jqsrt.2021.107529)

|  |
| --- |
| PART 1: Comments |
|  | Reviewer’s comment**Artificial Intelligence (AI) generated or assisted review comments are strictly prohibited during peer review.** | Author’s Feedback *(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)* |
| **Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.** | **This manuscript is an excellent discourse to undetstant molecular bonding and the relevant theories along with experimental references. The transition from strong covalent bond to weak vader-waal bond as function of vibronic quantum numbers is explained with excellence. The degrees of freedom of the** $Be\_{2}$ **molecule are described and its relation with bonding shown explicitly. Different potential models as EMO,MEMO, ab initio MRCI and other models have been explicitly shown through table. The bond strength have been detailed via Potential energy curve analysis with the bound state, metastable and stattering state where the metastability is described as a function of rotational quantum numbers. The Slater Type Orbitals (STO) described the basis sets have been represented in a prolific way and different polynomials have been inserted to make convergence. Moreover, internuclear distance between the dimer plays a vital role in deciding the bonding and its turning shows the transition from one bonding to another which is said to be the duel property by the author. Here the Born-Oppenheimer approximation is taken so that the dirrerent motions of the di-atomic model does get intertwined with each other.** **Moreover, this manuscript may contribute to molecular physics, quantum mechanics and condensed matter physics to a great extent. The ab initio model takes into account the many-body physics and along with Hartree-Fock method and Self consistennt field enriches the paper. Relativistic treatments in the higher energy regime also enriches the Physics that helps scientific community.** |  |
| **Is the title of the article suitable?****(If not please suggest an alternative title)** | **This manuscript contains information and analysis of chemical bond and spectrum of a diatomic molecule. The title given is good but might have been better if it had been given as-“Quantal Treatment of Dual Character of the Be2 molecule while forming bond in the X1** $Σ \_{g}^{+}$ **state”.** |  |
| Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here. | **The abstract is no doubt subtle and compact. Everything, starting from dual nature of bond, the present ab initio model, the morse potential, different bound states (stable, metastable and scattering) have been touched. The perspective of relativistic effect also has been summarised. Then, came the issue of final singularity also came naturally.****So, there is no saying about the abstract. Only, One or two application could have stated for better reproducibility.** |  |
| **Is the manuscript scientifically, correct? Please write here.**  | **The representation has been both artistic and scientific. It has eight sub-headings which are absolutely okay for the better understanding of the manuscript. 68 references have been given. Also the manuscript is endowed with relevant tables and graphical representations. I found no illogical statement anywhere in the article.**  |  |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.****-** | **There are 68 references. Diacronically it starts from 1920 to 3-4 years back from the present time. The old papers are highly necessary for literature review and gathering basic concepts. Actually, this article consists of less number of recent references which could have given some new and presently said models. But, it does not affect substanciably.** |  |
| Is the language/English quality of the article suitable for scholarly communications? | **The Enlish given here has a smooth ongoing. The is no mistake in grammar. Spellings are sound also.** |  |
| Optional/General comments | 1. Quantal treatment obviously promoted value of molecular description
2. The graphical descriptions: 1 &2 are mentionworthy
3. Computationally and numerically enriched to handle large number of rotational and vibronic quantum numbers.
4. The Slator Type Orbital (STO) has been relevant
5. The phase shift in case of scattering-energy graph gives better reproducibility
6. The analogy of laser principle has been quite matching with the metastable state.
7. The variance of vibrational constant with the vibrational quantum numbers made the article practically more stable.
 |   |

|  |
| --- |
| **PART 2:**  |
|  | Reviewer’s comment | Author’s comment *(if agreed with the reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)* |
| **Are there ethical issues in this manuscript?**  | *(If yes, Kindly please write down the ethical issues here in detail)* |  |

**Reviewers:**

**Subhajit Samaddar, India**