Review Form 3

Journal Name:	**Asian Journal of Chemical Sciences**
Manuscript Number:	**Ms_AJOCS_129275**
Title of the Manuscript:	**The Integration of Machine Learning and Predictive Modeling: A New Era in Computational Chemistry and Materials Science**
Type of the Article	**Review Article**

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This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty'**, provided the manuscript is scientifically robust and technically sound.
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PART 1: Comments

	Reviewer's comment	**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.	The manuscript overviews the lately developed efficient approaches needful to compute the materials properties in the limited computational resources. The exceptional workability of the integrative approaches of the ML schemes are presented. It is scientifically relevant, and informative to the wide range audiences. But, to some extents, the "for and against" logical interpretations presented for the ML and non-ML techniques are being lacked: it reflects that the wordy presentations are a little bit bias.	
Is the title of the article suitable? **(If not please suggest an alternative title)**	**Yes**	
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.	**Yes,** (in order to claim the advancements in the computing abilities, the quantitative performances are to be included to rate the qualifications of the integrative and non-integrative schemes to each other). After the author improvising few of the subsections suggested in the "PART 2: REVIWER'S COMMENTS", at least one to two lines to prioritize and forecast the applicative features of the former over the latter are expected in the abstract section.	
Is the manuscript scientifically, correct? Please write here.	**Yes** (if the author tries to include the suggestions given in the "PART 2: REVIWER'S COMMENTS" at most, the actual reviews and the related flavours are found throughout the manuscript.)	
Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.	**Yes,** (the ideological quantitative justifications and declarations are not taken from the cited resources so that the analogical interpretations are being missed a little bit)	
Is the language/English quality of the article suitable for scholarly communications?	**Yes**	
Optional/General comments	The overall evaluation marks this article publishable. However, the author is strongly suggested to incorporate the following constructive comments (PART 2) in order to make his/her article scientifically potent. The review article is generally inclusive with the critical views of the authors made on the bases of the literature datasets and therein presented quantitative analyses. For example, in some subsections, the author's remarks and the disparate performances of the integrative and non-integrative approaches are being lacked with the quantitative ratings and experimental/theoretical datasets.	

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)*
	1. In subsection 1.1, Traditional methods like density functional theory (DFT) and molecular dynamics offer valuable insights but are computationally expensive and require expertise: Please address that several DFT based methods are made efficient, versatile, yet accurate like DFTB+ (SCC and NCC DFTB). The more genuine reason of integrating ML algorithms to the DFT and *ab initio* principle are expected here. 2. In subsection 1.3, the author is advised to underscore the ML performances to ease the complexity associated with the MD/MM etc. simulation processes so that more concrete roles of the ML algorithms in computational/theoretical sciences are incorporated. 3. In subsection 3.1, "Solubility predictions rely on molecular descriptors": Please include few descriptors that practically describe QSPR features in theoretical chemistry, and link to what extents ML can address them (if any quantitative datasets are available, please rate the performances on the same bases). ML also identifies reactive sites and optimizes reaction conditions using attention mechanisms: Does the qualification of the ML lie into potential regime of *Gaussian* calculation framework? The quantitative disparate performances of them are needful to make the statement expressive.	

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	4. In subsection 3.3, the straightforward presentation makes something lacking there: In what accuracy range doe the ML produce the results that the author/s want to highlight here? For example, the modeling reaction pathways and mechanisms are even though predictive efficiently, but it would be better to rate it with the performances of the relevant model. 5. In subsection 4.1, ML is particularly valuable in designing energy materials, such as high-performance battery electrodes: since it is the review article, the quantitative information is sought out rather qualitative. The author/s are suggested to mention the few battery systems that actually employ the ML designed materials as electrodes, and exhibit the satisfactory performances if any. It really makes this article quite informative. 6. The subsections 4.2 to 4.4 are finely presented with illustrative examples. 7. In the subsection 5.1: the DFT-error minimizing skills of the ML in real time are presented, but lacks of "what are the negative and positive impacts of the ML integrated DFT towards unveiling the physicochemical properties in an acceptable accuracy range?" 8. In subsection 6.1 or 6.2, the author is suggested to include predictive ability of the ML methods even without the presence of high-quality datasets (primary sources). In what extents can the ML be trained and routed to predict the advanced properties without feeding the pre-calculated datasets?	
Are there ethical issues in this manuscript?	**No**	
Are there competing interest issues in this manuscript?	**No**	
If plagiarism is suspected, please provide related proofs or web links.	**No** (the editorial screening board is more responsible for this)	

PART 3: Declaration of Competing Interest of the Reviewer:

Here reviewer should declare his/her competing interest. If nothing to declare he/she can write "I declare that I have no competing interest as a reviewer"

I declare that I have no competing interest as a reviewer.

PART 4: Objective Evaluation:

Guideline	MARKS of this manuscript
Give OVERALL MARKS you want to give to this manuscript (Highest: 10 Lowest: 0) **Guideline:** Accept As It Is: (>9-10) Minor Revision: (>8-9) Major Revision: (>7-8) Serious Major revision: (>5-7) Rejected (with repairable deficiencies and may be reconsidered): (>3-5) Strongly rejected (with irreparable deficiencies.): (>0-3)	 7 9 0 (NO) 0 (NO) 0 (NO REJECTION) 0 (NO REECTION)

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Editorial Comments (This section is reserved for the comments from journal editorial office and editors):

	Author's Feedback

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