

Response to reviewer 2

Reviewer 2:

The manuscript 'Computational Assessment of Steric and Electronic Contributions in Stereoselective Olefin Polymerization by Nonmetallocene Catalysts' is the trial to analyze the influence of structural elements for the stereoselectivity of propene polymerization promoted by nonmetallocene systems using computational approach. The paper sounds interesting for the potential reader, but some improvements are needed before publications in 'Molecules' journal.

Our reply:

We thank the reviewer for the nice comments. The minor issues have been updated. As a matter of fact, a thorough revision of the whole manuscript has been done and we thank this reviewer for his/her kind advices. Some of the main aspects are reported point-by point.

COMMENTS:

The abstract should be rewritten. There is a need to add the motivation of the research, the goal and 2-3 sentences regarding the main findings. The description of the methodologies should be moved to introduction section.

Our reply:

We thank the reviewer for the observations. The abstract was completely rewritten with a special emphasis on the motivation and goals of our work.

COMMENTS:

The English language should be checked from grammar point of view

Ln 94 – Computational details section should be replaced by the word 'Methodology' and should be visualized as a pipeline to make the description understandable by the potential reader.

Our reply:

The English language has been checked from the grammar; the computational details section has been replaced by the word Methodology and a new Scheme, (See Scheme 2 of the revised version) has been added as a pipeline.

COMMENTS:

The introduction – clearly define the scientific impact of the research. The description regarding different methods for the propene stereoselectivity should be added as well as assessment issues.

Our reply:

In the revised version we better defined the reason why we selected this particular class of catalysts stressing the peculiar molecular architecture not accessible to other catalytic systems. Furthermore, during the manuscript, we focused better the vantages of the combined approach by using DFT *and* %V_{Bur} *and* ASM-NEDA analysis.

COMMENTS:

The description of all materials, software, hardware, statistical tools should be added as well as clear description of the analyzed experimental data set (link to the date will be preferred as well)

The statistics should be added for obtained results, as well as a computational aspects.

Figure 1 – 2 – data for systems IIe should be added

Our reply:

All the calculations requested by the reviewer on the system IIe have been added as well as the % V_{Bur} steric maps and the ASM-NEDA analysis.

COMMENTS:

Figure 3 – the description of the scale is needed.

Our reply:

The revised caption of the Figure 3 has been completed with the description requested by the reviewer.

COMMENTS:

In the discussion section the comparison between method used for the assessment is needed. Additionally the importance of the obtained results should be added. The advantages and disadvantages of the analyzed systems regarding introduced assessment should be described and analyzed as well. Results should be described in more understandable and systematic way.

Steric maps (fig and 6) should be presented for all analyzed systems (one figure) as well as DFT optimized geometries. This can make the analysis of the results easier.

Our reply:

We followed the indications of the reviewer. All the systems reported have been analyzed and discussed. We compacted the % V_{Bur} in a single Figure and the remaining systems in the Supporting Informations. However, we preferred to use several figures for the DFT optimized geometries for the sake of readability because they are discussed in different part of the text.

COMMENTS:

The conclusion should be rewritten. Please include main findings corresponding to the title – computational assessment. The conclusion should consist of clear description of the added value of the research. Current version would confuse the reader

Our reply:

We rewrote completely the conclusion following the reviewer suggestions.