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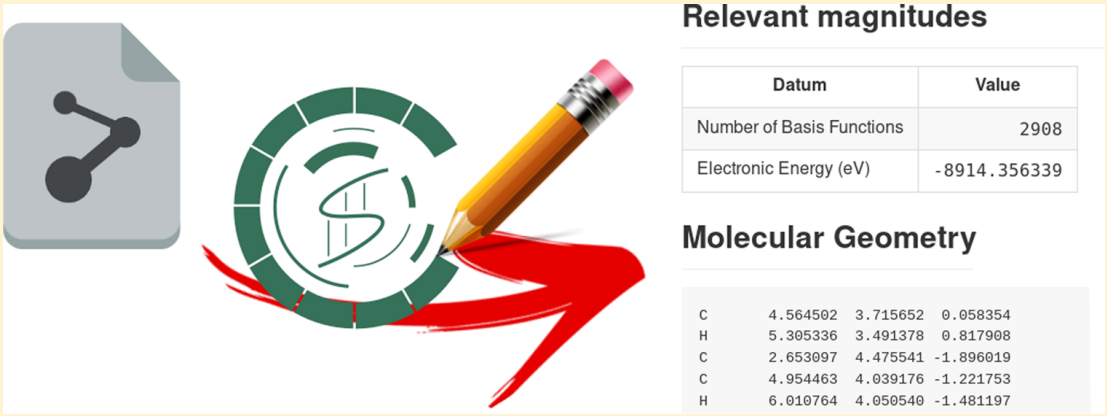
ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications

Jaime Rodríguez-Guerra Pedregal,* Pablo Gómez-Orellana, and Jean-Didier Maréchal*

Departament de Química, Universitat Autònoma de Barcelona, 08193 Bellaterra (Barcelona), Spain

Supporting Information



ABSTRACT: Electronic supporting information (ESI) occupies a fundamental position in the way scientists report their work. It is a key element in lightening the writing of the core manuscript and makes concise communication easier for the authors. Computational chemistry, as all fields related to structural studies of molecules, tends to generate huge amounts of data that should be inserted in the ESI. ESI reports originating from computational chemistry works generally reach tens of sheets long and include 3D depictions, coordinates, energies, and other characteristics of the structures involved in the molecular process understudy. While most experienced users end up building scripts that dig throughout the output files searching for the relevant data, this is not the case for users without programming experience or time. Here we present an automated ESI generator supported by both web-based and command line interfaces. Focused on quantum mechanics calculations outputs so far, we trust that the community would find this tool useful. Source code is freely available at https://github.com/insilichem/esigen. A web app public demo can be found at http://esi.insilichem.com.

INTRODUCTION

One of the major exercises with which scientists are confronted is to write articles in a concise, direct, and convincing manner. This exercise is only possible if the core manuscript presents the most important concepts, results, and discussions while technical details and further analysis are part of additional documents. Supporting information (SI) and its electronic counterpart (ESI) represent a key asset in scientific communication. SI reports allow researchers to provide details on their studies so that reviewers and readers can assess the quality of the practices and reach relevant information to reproduce or apply them in the context of their own investigation. It is therefore a common procedure to submit extensive SI documents along the main manuscript; something that is highly supported by scientific journals, which provide specific contexts and guidelines for this process.

In computational chemistry, at least two challenges exist in the generation of SI documents. The first one is the handling of massive amounts of data. For example, the mechanistic study of a chemical reaction likely includes 3D representations for the reactants, products, and relevant intermediates for the paths under study, as well as text data like energies, stoichiometry, or transition state vectors, at least. These data are normally scattered in complexly structured output files, and the second challenge consists therefore in gathering them efficiently. Researchers with the convenient programing skills generally end up building scripts to generate their SI documents. Those go over the output files, search for the relevant data, and write it an (un)formatted file that is finally pasted in a more advanced text processor. When developing new scripts, one could bet on available programs and libraries to handle the parsing[1−4] and then simply focus on the style of output format. However, users without programming experience will avoid the technical complexities involved and become experts in copy−pasting exercises: a cumbersome handcrafting process easily prone to human error.

While there are several software projects that could be helpful in this task, such as spreadsheet automation,[5] desktop graphical interfaces for results analysis (GaussView,[6] GaussSum[1]), or custom database creation (GaussDal,[7] MyChem[8]), they mainly operate as standalone data collectors. In the end,

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