

Accepted Manuscript

Gaussian Basis Implementation of the Charge Patching Method

Zarko Bodroski, Nenad Vukmirović, Srdjan Skrbic

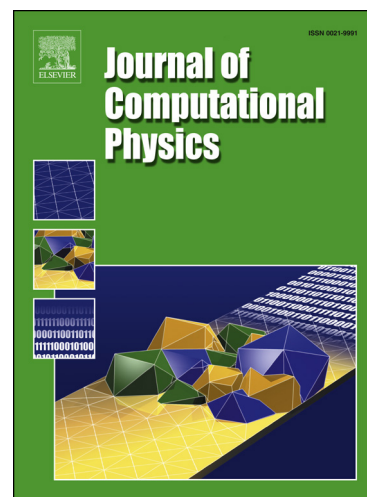
PII: S0021-9991(18)30257-2
DOI: <https://doi.org/10.1016/j.jcp.2018.04.032>
Reference: YJCPH 7972

To appear in: *Journal of Computational Physics*

Received date: 6 October 2017
Revised date: 5 April 2018
Accepted date: 17 April 2018

Please cite this article in press as: Z. Bodroski et al., Gaussian Basis Implementation of the Charge Patching Method, *J. Comput. Phys.* (2018), <https://doi.org/10.1016/j.jcp.2018.04.032>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Highlights

- Efficient numerical implementation of charge patching method is presented.
- Wave functions and charge density are represented using Gaussian basis sets.
- Charge density motifs represented on a real-space uniform grid.
- One thousand atoms systems can be calculated on a single CPU core in several hours.

Download English Version:

<https://daneshyari.com/en/article/6928755>

Download Persian Version:

<https://daneshyari.com/article/6928755>

[Daneshyari.com](https://daneshyari.com)