# QM-like partial atomic charges for AlphaFold available online

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Proteins are the basic functional unit of all living organisms. Critical information for understanding the function of a protein is its structure. Thanks to the AlphaFold algorithm [1], which predicts structure based on sequence, the number of predicted structures is growing very rapidly. Unfortunately, due to the computational complexity, we are unable to directly calculate the second key characteristic, i.e., electron density, for such large structures. A suitable approximation is the concept of partial atomic charges, which describe how much electron density belongs to each protein atom. Partial atomic charges can be derived directly from the electron density or might be calculated by fast empirical methods. However, these methods must go through a parameterization process, during which the parameters of an empirical method are optimized to reproduce the charges from quantum mechanics (QM).

This work introduces an empirical method called Split-charge equilibration with parameterized initial charges (SQE+qp) [2] adapted for AlphaFold Protein Structure Database. Our method can reproduce QM partial atomic charges with high accuracy. We also present an implementation of SQE+qp and its parameters via a web application Atomic Charge Calculator II [3] at [https://acc2.ncbr.muni.cz](https://acc2.ncbr.muni.cz/). Thus, we provide the scientific community with a freely available online tool for calculating QM-like partial atomic charges.

[1] Varadi, M *et al*. AlphaFold Protein Structure Database: massively expanding the structural coverage of protein-sequence space with high-accuracy models. *Nucleic Acids Research* (2021).

[2] Schindler, O *et al.* Optimized SQE atomic charges for peptides accessible via a web application. *Journal of Cheminformatics* (2021).

[3] Raček, T *et al.* Atomic Charge Calculator II: web-based tool for the calculation of partial atomic charges. *Nucleic Acids Research* (2020).