BIAC.py: Python code to display Bond Indices and Atomic Charges on VMD

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The visualization properties computed with much computational chemistry software (MOPAC, Gaussian, ORCA, etc.) has always been a difficult challenge for many users who do not have the necessary computational skills to represent these results in an orderly way or high-quality images, especially the representation of charges or bond indices. The main objective of this work is to show a python code to represent clearly and visually the bond indices and atomic charges of quantum chemistry calculations in Visual Molecular Dynamics (VMD); this will facilitate the visualization and representation of the data obtained from the computational calculations. The program visualizes charges of the NPA, Mulliken, ESP, RESP, etc. type and Wiberg bond indexes. Currently, the program reads MOPAC, Gaussian, and ORCA results to represent partial charges or bond indices.

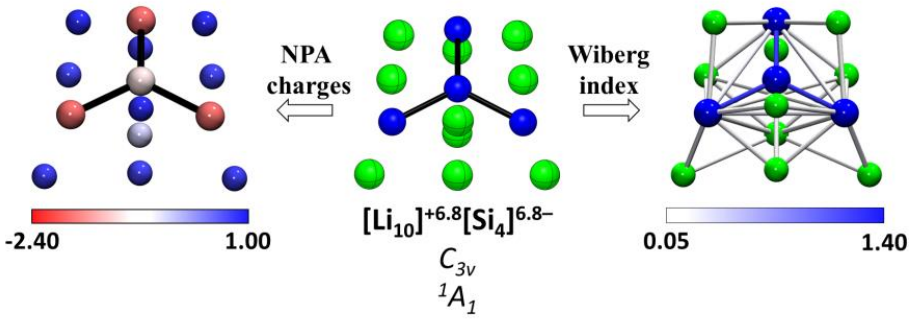

Figure 1: NPA charge and WBI values for $Li_{10}Si_4$

Acknowledgments: Powered@NLHPC: This research was partially supported by the supercomputing infrastructure of the NLHPC (ECM-02).