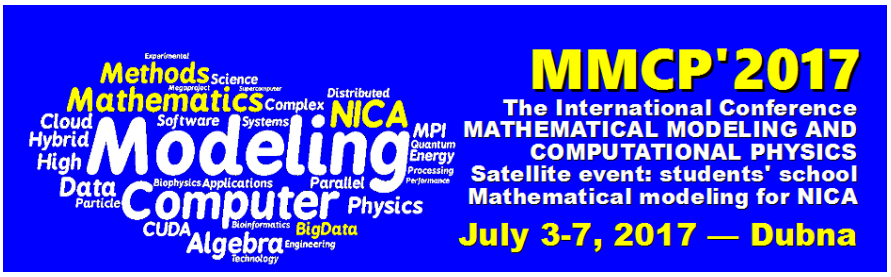

Contribution ID: **10** Type: **not specified**

A new orbital free simulation method based on the density functional theory

We propose a practical way to simulate multi-atomic systems without using of wave functions (orbitals). Our approach is based on the theoretical concept of the last years (FTT 2012, Sarry AM, Sarry MF; JETP 2013, Bobrov VB, Trigger SA) claiming that the universal functional of kinetic energy does not exist. We construct kinetic functionals for each type of atoms and then use them for complex systems. On examples of clusters containing Al, Si, C, and O we have shown that our method can describe structures and energies of multi-atomic systems not worse than the Kohn-Sham method but faster.

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