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**Wavelets and Evolutionary Algorithms on the Eletronic Wavefunctions.** IURY STEINER BEZERRA, PUC- Rio, MARCO AURELIO PACHECO, PUC-Rio — The simulation of the electronic structure of atoms and molecules has been shown to be, from the beginning of 90's, an indispensable tool for the development of strategic areas, that are still emergent, but fundamental, like nanotechnology. However, this type of simulation is still of great complexity today and demands high computational power. Thus, the creation of more precise and less costly methods becomes fundamental. With the elaboration of this research, the intention is to create alternatives basis that can be used in the traditional methods of simulation of electronic structure, such as the Hartree-Fock method, GVB, among others. This essay show new developments used in the calculations of electronic structure, in order that can create disruptive approaches, related to the precision or velocity of the obtainment of relevant results. The new methods are based on Computational Intelligence and concepts of Functional Analysis like Wavelets. Here, the wavelet series is considered a particular case of Fourier Series, where the basis for linear space is a set of wavelet functions. Here is introduced a fast way to use wavelet in analytic calculations and a is built a new kind of linear basis.

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