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Quantum Inspired Evolutionary Algorithm applied to the optimization of Basis Functions

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Abstract – Nanoscience and Nanotechnology development are strongly dependent upon the advancement of Computational Chemistry. Solutions for Schrödinger's equation rely basically on the important concept of Basis Functions. The goal of this work is to create improved Basis Functions, looking forward to get better results for basic quantities as the total energy of a quantum system using a methodology based on Quantum Inspired Evolutionary algorithms.

Basis Functions consist of a set of functions that, linearly combined, approximate the exact solution of Schrödinger's electronic equation. The project and parameterization of Basis Functions is a hard task which influences the computational cost and result's precision of the electronic structure calculus [1]. For those atoms that have symmetries other than *s*, there is a greatest difficulty associated to the project of Basis Functions. Besides the search for an optimum parameterization of each primitive, it is also necessary that the functions be correctly distributed among the existent symmetries on the studied system.

Conventional techniques of non-linear programming have been extensively used to parameterize Basis Functions [2], but cannot be used to specify the distribution of primitives present on each symmetry. The main advantage of using evolutionary techniques is the ability to achieve good solutions for both discrete and continuous non-linear problems. In addition, the previous knowledge of an initial solution to the problem is not necessary.

The main procedure consists in evaluating a set of parameters conducted by Quantum Inspired Evolutionary Algorithm (*QIEA*) in towards a global minimum, taking care to distribute s and p number of functions with respect to problem's symmetries.

QIEA is a new kind of Evolutionary Algorithm that uses probability distributions for each free variable of the problem, in order to simulate the superposition of solutions, which is intrinsic in the quantum computing methodology.

This work evaluated different ways to implement the design of the Basis Functions with nature inspired techniques together with polynomial expansions. These expansions are used with the purpose of reducing the dimensionality of the search space. For atoms which have s and p symmetries, the main results achieved were significantly better than those presented in literature [4], and a few results are shown on table 1.

Table 1: Energy differences with respect to numerical calculations (ΔE in microhartrees) in this work and Klubowski [4] for Ar atom.

Total of basis	QIEA 1			Ref [4]			Improvement
20	21371.602	12s	8p	45972	13s	7p	53.51%
22	7811.709	13s	9p	14444	14s	8p	45.92%
24	2991.478	14s	10p	5035	15s	9p	40.59%
26	1215.931	15s	11p	1838	16s	10p	33.84%
28	532.487	16s	12p	666	17s	11p	20.05%
30	243.511	17s	13p	259	18s	12p	5.98%
32	102.042	18s	14p	105	19s	13p	2.82%
34	41.093	20s	14p	44	20s	14p	6.61%
36	17.482	21s	15p	20	21s	15p	12.59%

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