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Three dimensional time dependent Schrödinger equation solver for multiple charge center systems NICOLAS BIGAOUETTE, EDWARD ACKAD, LORA RAMUNNO, University of Ottawa — We extended a method to solve the time dependent Schrödinger equation in 3D [1] to study multi charge centers in the single active electron approximation. It is based on a well-known computational electromagnetism algorithm called Finite-Difference Time-Domain. Our method can be used both to solve for the electronic wavefunctions in an arbitrary potential shape (independent of the presence of any symmetry), and to calculate the solution of time-dependent systems. As a first step, we verify our method by solving for the eigenstates of the H_2^+ molecule. Further, we investigate more complicated multicore systems, such as small charged atomic clusters.

[1] I W. Sudiarta et. al. J. Phys. A 40 (2007) 1885

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