

real-time dynamics of atoms and/or molecules in a strong laser field. Incorporation of other pseudopotentials more suited to DFT as well as more extended and elaborate basis sets would be among some of the important issues which may be considered in recent future. More accurate XC functionals could also be employed depending upon the physical system concerned and the nature of the problem dealt with. Applications to weakly bonded systems, clusters and of course, to larger systems would further consolidate its success. Finally although one could think of some inherent errors associated with the incompleteness of the grid, this study confirms that with a judicious choice of the grid coupled with a correct treatment of the Coulomb potential, these can be reduced to tolerable minima. Thus very satisfactory results could be obtained.

Acknowledgments

The project was initiated at Prof. D. Neuhauser's laboratory at the Univ. of California, Los Angeles, where the core of the program was written. It was further extended at Prof. S. I. Chu's laboratory at the University of Kansas. I thank them for stimulating discussions and providing the computational facilities. Numerous useful discussions with Dr. E.I. Proynov is gratefully acknowledged. Warm hospitality offered by UCLA and the Univ. of Kansas is greatly appreciated. An anonymous referee is thanked for valuable constructive comments.

-
- [1] S. R. White, J. W. Wilkins and M. P. Teter, Phys. Rev. B **39**, 5819 (1989).
 - [2] J. R. Chelikowsky, N. Troullier, K. Wu and Y. Saad, Phys. Rev. B **50**, 11355 (1994).
 - [3] E. L. Briggs, D. J. Sullivan and J. Bernholc, Phys. Rev. B **52**, R5471 (1995).
 - [4] F. Gygi and G. Galli, Phys. Rev B **52**, R2229 (1995).
 - [5] T. L. Beck, Rev. Mod. Phys. **72**, 1041 (2000).
 - [6] T. Helgaker, P. Jorgensen and J. Olsen, *Molecular-Electronic Structure Theory* (John-Wiley & Sons Ltd., 2000).
 - [7] M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias and J. D. Joannopoulos, Rev. Mod. Phys. **64**, 1045 (1992).