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Ahlrichs R, Penco R & Scoles G. Intermolecular forces in simple systems. *Chem. Phys.* 19:119-30, 1977.
[Institut für Physikalische Chemie, Univ. Karlsruhe, Federal Republic of Germany; Facoltà di Scienze, Libera Univ. Trento, Povo, Italy; and Guelph-Waterloo Centre Grad. Work in Chemistry, Univ. Waterloo, Ontario, Canada]

This paper assessed the reliability of a previously proposed method to describe in a simple way the weak van der Waals interaction between nonbonded systems, such as rare gas atoms. [The *SCI*® indicates that this paper has been cited in over 190 publications.]

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Credit for this article must be given to Giacinto Scoles, who had the idea and pushed the work. From his experimental work, he was interested in intermolecular interactions and had worked out a new method[1] to predict them. This approach, called HFD for Hartree-Fock-Dispersion, combined information from *ab initio* HF calculations (describing repulsive forces) with an empirical estimate of attractive dispersion terms. The latter were multiplied by a damping function F (to rectify certain problems), which Scoles believed to be "universal."

I first met Scoles at a conference in Boulder in 1975 (I do not remember having met R. Penco), as he recalls since I had forgotten the occasion. But, I do remember our discussions. Scoles, an energetic Italo-American, was fascinated by his idea, but theoreticians, including myself, were not. We did not like the elements of empiricism in the HFD approach and could not see why the very same function F should apply to all cases.

All that Scoles needed to further test and establish his method were accurate approximations for potential curves of Ne_2 and other rare gas systems within the HF method. This, together with more reliable dispersion coefficients that had just become available, would allow for a thorough check of the HFD method. Although I could easily have done the calculations needed and although I was interested in the field, I remained reluctant. I could not imagine that such a simple method would work. But Scoles did not give up. He kept in touch with me, even visited me in Karlsruhe, and I did my homework too, which required a week or two only. The effort was worthwhile and confirmed Scoles's ideas: HFD provided a surprisingly accurate description for the cases considered.

When I met Scoles again some years later, he said, "This is probably the most-quoted paper of yours and you still don't quite believe in it." The point is that the HF calculations I did were rather trivial to me—almost boring. I would have preferred to perform rigorous calculations that were not possible then and are still demanding today. Scoles was aware of the problems encountered in purely theoretical treatments, but he fully realized the great need to develop and test approximate treatments that would be of great help, as the numerous citations to our paper show.

The HFD method was later refined by Scoles and coworkers.[2] Another successful approach to predict semiempirical potentials was worked out by K.T. Tang and J.P. Toennies.[3] Together with my students, I have recently developed a method—again based on a combination of *ab initio* and experimental data—to treat interaction between molecules[4] that still uses ideas of the "Ahlrichs-Penco-Scoles paper." [Editor's note: A recent review on van der Waals molecules has been published by A.D. Buckingham, P.W. Fowler, and J.M. Hutson.[5]]

1. **Hepburn J, Scoles G & Penco R.** A simple but reliable method for the prediction of intermolecular potentials. *Chem. Phys. Lett.* 36:451-6, 1975. (Cited 65 times.)
2. **Douketis C, Scoles G, Marchetti S, Zen M & Thakkar A J.** Intermolecular forces via hybrid Hartree-Fock-SCF plus damped dispersion (HFD) energy calculations. An improved spherical model. *J. Chem. Phys.* 76:3057-63, 1982. (Cited 75 times.)
3. **Tang K T & Toennies J P.** An improved simple model for the van der Waals potential based on universal damping functions for the dispersion coefficients. *J. Chem. Phys.* 80:3726-41, 1984. (Cited 65 times.)
4. **Böhm H J, Ahlrichs R, Scharf P & Schiffer H.** Intermolecular potentials for CH_4, CH_3F, CHF_3, CH_3Cl, CH_2Cl_2, CH_3CN and CO_2. *J. Chem. Phys.* 81:1389-95, 1984. (Cited 25 times.)
5. **Buckingham A D, Fowler P W & Hutson J M.** Theoretical studies of van der Waals molecules and intermolecular forces. *Chem. Rev.* 88:963-88, 1988.

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