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New Methods for Tackling Large Systems

Prof. Alain St-Amant
Department of Chemistry, University of Ottawa

The research efforts of our group concentrate mainly on the development of new approaches ultimately geared towards the accurate modeling of enzymatic reactions. These systems require the development of new methods that will allow us to tackle such large molecular systems. These advances are being implemented within our own research group's density functional software package. Following a brief description of the conventional methodology, we will present recent advances in linear scaling methods, coupled QM/QM methods, coupled QM/MM methods, and the inclusion of thermal effects by hybrid Monte Carlo and molecular dynamics approaches.

Alain St-Amant graduated in 1986 from University of Winnipeg. He pursued his M.Sc. and a PhD in Theoretical Chemistry at Université de Montréal with Dennis Salahub as an NSERC graduate fellow. He then crossed the border and was an NSERC Postdoctoral Fellow with Peter Kollman at University of California, San Francisco from 1992 to 1993. Dr. St-Amant returned to Canada in 1993 and joined the Department of Chemistry at University of Ottawa, where he is now an Associate Professor. Dr. St-Amant is a co-author of the deMon suite of computer programs and his group is actively developing the DeFT computer package.