

CURRICULUM VITAE

1. Personal Details

Name: Inge Røeggen

Date of Birth: June 22 1942

Nationality: Norwegian

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2. University Education

- (1) Cand. mag., University of Oslo, Oslo, Norway, 1966
- (2) Cand. real., University of Oslo, Oslo, Norway, 1968
- (3) Dr. philos., University of Oslo, Oslo, Norway, 1972

3. Employment Records

- (1) Research assistant, Institute of physics, University of Oslo, Oslo, Norway, 1969-1972
- (2) Associate professor, Institute of mathematical and physical sciences, University of Tromsø, Tromsø, Norway, 1974-1991
- (3) Professor, Institute of mathematical and physical sciences, University of Tromsø, Tromsø, Norway, 1991

4. Sabbatical Leave

- (1) Department of Theoretical Chemistry, University of Oxford, Oxford, England, 1973-1974
- (2) Institute for Molecular Science, Okazaki, Japan, 15.01.87-15.06.87
- (3) Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, USA, 11.05.93-06.12.93
- (4) I.R.S.A.M.C., Laboratoire de Physique, Université Paul Sabatier, Toulouse, France 1.02.98-15.12.98
- (5) I.R.S.A.M.C., Laboratoire de Physique, Université Paul Sabatier, Toulouse, France 1.09.03-30.05.04

5. Research Interests

- (1) The electron correlation problem in molecules and molecular complexes
- (2) Intermolecular interactions
- (3) Presently I am working on a new conceptual and computational

model for describing the electronic structure in molecules and solids: the PATMOS model (Perturbed Atoms in Molecules and Solids). A key element in this approach is the definition of a perturbed atom in the complex. The perturbed atom is at the lowest level described by an UHF-function(The UHF orbitals are localized). Energy corrections are calculated according to the energy incremental scheme. In the calculation of intra- and interatomic energies, model systems are introduced. To each atom is associated a set of partner atoms defined by a vicinity criterion. In the independent calculations of intra -and interatomic energies, the calculations are performed on model systems comprising the atoms considered and their partner atoms.

6. Publications (refereed journal articles)

If the author(s) is not specified for a paper in the list of publications, I am single author.

1. The Theory of the Stark effect in multiplet states of diatomic molecules.
J. Phys. B: Atom. Molec. Phys. **4**, 168 (1971).
2. On the Determination of Small Electric Dipole Moments of Excited Electronic States in Diatomic Molecules.
J. Mol. Spectrosc. **39**, 123 (1971).
3. Polynomial Approximations to the stark perturbed Rotational Energy levels of the Rigid Symmetry Top Rotor.
Atomic Data **4**, 289 (1972).
4. On the Calculation of permanent Electric Dipole Moments and Polarizability Anisotropies from Stark Effect Data.
J. Mol. Spectrosc. **44**, 470 (1972).
5. The Inversion Eigenvalues of Non- Σ States of Diatomic Molecules, Expressed in Terms of Quantum Numbers.
Theoret. Chim. Acta (Berl.) **21**, 398 (1971).
6. On least Squares Estimation of Non-Linear Parameters with Particular Emphasis on Matrix Evaluation.
Physica Norvegica **7**, 33 (1973).
7. On the Quantization of Angular Momenta in Diatomic Molecules.
Physica Norvegica **2**, 161 (1974).
8. Convergence Acceleration of matrix Hartree-Fock Calculations by Padé Approximants of Type II.
Chem. Phys. Letters **22**, 140 (1973).
9. Applications of Padé Approximants of Type II in Partitioning Technique.
Int. J. Quant. Chem. **7**, 1193 (1973).
10. Resolvent technique and Padé Approximants in Configuration Interaction Calculations.
Int. J. Quant. Chem. **9**, 431 (1975).
11. Application of a Least-Squares method in Configuration Interaction Calculations.
Chem. Phys. Letters **31**, 271 (1975).

12. I. Røeggen, J.P. Huggett and E.A.G. Armour:
A Least-Squares Method Applied to the Hydrogen Molecule.
Theoret. Chim. Acta **39**, 161 (1975).
13. I. Røeggen and K. Aashamar:
Pair functions and biorthonormal orbitals in the context of
the method of moments. I.
Molec. Phys. **33**, 453 (1977).
14. Antisymmetric Product of Geminals in the Context of the
method of Moments.
Int. J. Quant. Chem. **19**, 319 (1981).
15. Electron Correlation Described by an Extended Geminal Model.
Int. J. Quant. Chem. **20**, 817 (1981).
16. Electron Correlation Described by Extended Geminal Models:
The EXGEM2 and EXGEM3 Models.
Int. J. Quant. Chem. **22**, 149 (1982).
17. An Extended Geminal Model Calculation of the Dissociation
Energy of the Ground State of Li_2 .
Chem. Phys. Letters **92**, 398 (1982).
18. Electron correlation described by an extended group function
model: The EXGF1 model.
J. Chem. Phys. **78**, 2485 (1983).
19. Derivation of an extended geminal model.
J. Chem. Phys. **79**, 5520 (1983).
20. Intermolecular potentials calculated by an extended geminal
model: Theory.
J. Chem. Phys. **85**, 262 (1986).
21. On the weaknesses of the VSEPR model.
J. Chem. Phys. **85**, 969 (1986).
22. I. Røeggen and E. Wisløff-Nilssen:
The Beebe-Linderberg two-electron integral approximation.
Chem. Phys. Letters **132**, 154 (1986).
23. I. Røeggen and E. Wisløff-Nilssen:
An energy fragment analysis of molecular properties: Theory.
J. Chem. Phys. **86**, 2869 (1987).
24. Electron Correlation Described by Extended Geminal Models:
The EXGEM4 and EXGEM5 Models.
Int. J. Quantum Chem. **31**, 95 (1987).
25. I. Røeggen, K. Morokuma and K. Yamashita:
On the binding energy of the ground state of Be_2 .
Chem. Phys. Letters **140**, 349 (1987).
26. Electron Correlation Described by Extended Geminal Models:
J. Chem. Phys. **89**, 441 (1988).
27. I. Røeggen and E. Wisløff-Nilssen:
Prediction of a metastable D_{3h} form of tetra oxygen
Chem. Phys. Letters **157**, 409 (1989).

28. Electron Correlation Described by Extended Geminal Models: The EXGEM7 and EXRHF3 Models. *Int.J. Quantum Chem.* **37**, 585 (1990).
29. Analysis of Hydrogen Bonded Systems: $(\text{H}_2\text{O})_2$, $\text{H}_2\text{O}\cdot\text{HF}$, $(\text{HF})_2$. *Mol.Phys.* **70**, 353 (1990).
30. Atoms and Electron-pair Bonds in a Molecule: An Approach within the Context of Extended Geminal Models. *Int. J. Quantum Chem.* **40**, 149 (1991).
31. I.Røeggen and T.Dahl:
An analysis of Weakly bonded EDA Complexes: F_2NH_3 , Cl_2NH_3 , CIFNH_3 . *J.am.Chem.Soc.* **114**, 511 (1992).
32. An Analysis of Electron Donor-Acceptor Complexes: BH_3CO , BH_3HN_3 . *Chem.Phys.* **162**, 271 (1992)
33. An energy decomposition analysis of intermolecular interactions. *J.Math.Chem.* **10**, 205 (1992).
34. I.Røeggen and H. Skullerud:
The interatomic potential for the $X\ ^1\Sigma$ state of NeLi^+ . *J.Phys.B:At.Mol.Phys.* **25**, 1795 (1992)
35. H.Skullerud, I.Røeggen and T.H.Løvaas:
Mobility and diffusion of lithium in neon
J.Phys.B: At.Mol.Phys. **25**, 1811 (1992)
36. I.Røeggen and P.Wind:
A theoretical study of the H_2 dimer: I.Bonding. *Chem.Phys.* **167**, 247 (1992)
37. P.Wind and I.Røeggen:
A theoretical study of the H_2 dimer: II. The potential energy surface. *Chem. Phys.* **167**, 263 (1992)
38. P. Wind and I. Røeggen: A theoretical study of the $(\text{H}_2)_2$ dimer. III. The isotropic potential. *Chem. Phys.* **174**, 345 (1993).
39. I. Røeggen, G. R. Ahmadi and P. A. Wind:
Intermolecular potentials calculated by an extended group function model: Theory. *J. Chem. Phys.* **99**, 277 (1993).
40. I. Røeggen and G. R. Ahmadi:
A quantchem chemical study of the F- and H-bonded isomers of HF/ClF . *J. Molec. Structure. (Theochem)* **307**, 9 (1994).
41. G. R. Ahmadi and I. Røeggen:
The interatomic potential for the $X\ ^1\Sigma$ state of ArLi^+ . *J. Phys. B: At. Mol. Opt. Phys.* **27**, 5603 (1994)
42. I. Røeggen, J. Almlöf, G. R. Ahmadi and P. A. Wind:
An accurate computational model for the study of intermolecular interactions. *J. Chem. Phys.* **102**, 7088 (1995)
43. I. Røeggen and J. Almlöf:
An accurate calculation of the three-body potential for the ground

- state of the helium trimer.
J. Chem. Phys. **102**, 7095 (1995)
44. G. R. Ahmadi, J. Almlöf and I. Røeggen:
The interatomic potential for the X $^1\Sigma$ state of ArNa⁺, NeNa⁺, HeNa⁺.
Chem. Phys. **199**, 33 (1995)
45. P. Wind and I. Røeggen:
Energy expansion in the extended geminal model.
Chem. Phys. **206**, 307 (1996)
46. I. Røeggen and J. Almlöf:
Interatomic Potential for the X $^1\Sigma^+$ State of Be₂.
Int. J. Quantum Chem. **60**, 453 (1996)
47. T. Dahl and I. Røeggen:
An Analysis of Electron Donor-Acceptor Complexes:
H₂OF₂, H₂OCl₂, and H₂OClF.
J. Am. Chem. Soc. **118**, 4152 (1996).
48. I. Røeggen and P. Wind:
Electron correlation, extended geminal models, and intermolecular
Interactions: Theory
J. Chem. Phys. **105**, 2751 (1996).
49. P. Wind and I. Røeggen:
Ab initio calculation of the three-body interaction in the (H₂)₃ trimer.
Chem. Phys. **211**, 179 (1996).
50. I. Røeggen and J. Almlöf:
An extended geminal calculation of the three-body potential for the
ground state of the helium trimer.
J. Molec. Structure. (Theochem) **388**, 331 (1996).
51. G. R. Ahmadi and I. Røeggen:
A minimal distortion localization of occupied orbitals in supermolecule
Calculations of intermolecular interactions.
Theor. Chem. Acc. **97**, 41 (1997).
52. Extended geminal models.
I. Røeggen, in Topics in Current Chemistry, **203**, 89 ,
Ed. P. R. Surján (Springer Verlag, Berlin, 1999).
53. M. T. Elford, I. Røeggen and H. R. Skullerud:
Interaction potential and transport coefficients for Li⁺ ions in helium.
J. Phys. B: At. Mol. Opt. Phys. **32**, 1873 (1999).
54. I. Røeggen, H. R. Skullerud, T. H. Løvaas and D. K. Dysthe:
The Li⁺ - H₂ system in a rigid rotor approximation: potential energy
Surface and transport coefficients.
J. Phys. B: At. Mol. Opt. Phys. **35**, 1707 (2002).
55. I. Røeggen and L. Veseth:
Interatomic Potential for the ground state of Be₂, Revisited.
Int. J. Quantum Chem. **101**, 201 (2005).
56. An ab initio study of the fcc and hcp structures of helium.
J. Chem. Phys. **124**, 184502 (2006).
57. An extended group function model for intermolecular interactions.
Theor. Chem. Acc. (2006)

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