# REAKTIVITAS ION KALSIUM(II) DALAM AMONIAK CAIR: STUDI SIMULASI DINAMIKA MOLEKULER *QUANTUM MECHANICAL CHARGE FIELD* (QMCF)

Wiji Utami

14/373104/PPA/04947

## INTISARI

Telah dipelajari reaktivitas ion $Ca^{2+}$ dalam amoniak cair menggunakan metode DM-QMCF. Metode DM-QMCF merupakan konsep perhitungan yang membagi dua daerah perhitungan. Daerah pertama mengandung spesi kimia seperti ion dan kulit solvasinya yang dihitung menggunakan mekanika kuantum, sementara daerah sisanya dihitung secara klasik. Tujuan penelitian ini adalah untuk mempelajari reaktivitas ion $Ca^{2+}$ dalam amoniak cair menggunakan metode simulasi dinamika molekuler QMCF. Sifat struktur dan dinamika diperoleh dari analisis fungsi distribusi radial, distribusi bilangan koordinasi, fungsi distribusi angular, waktu tinggal rata-rata ligan dan frekuensi vibrasi ion-amoniak.

Metode *ab initio* HF/SV(P) dan DZP Dunning divalidasi dengan menghitung energi BSSE. Sistem kotak simulasi diekuilibrasi selama 3 ps pada suhu 235,15 K, kemudian dilanjutkan dengan pengambilan data setiap tahapan kelima simulasi selama 12 ps. Hasil penelitian menunjukkan bahwa kulit solvasi pertama bersifat labil dan teramati mengandung 7 hingga 8 ligan amoniak. Waktu tinggal rata-rata ligan pada kulit solvasi pertama adalah 14,45 ps menunjukkan terjadi sedikit pertukaran ligan dengan kulit solvasi kedua. Hasil simulasi menunjukkan data yang mendekati dengan penelitian secara eksperimental dan teoritikal sebelumnya.

Kata kunci: amoniak cair, ion $Ca^{2+}$, DM-QMCF, reaktivitas

# *REACTIVITY OF CALCIUM(II) ION IN LIQUID AMMONIA: MOLECULAR DYNAMICS SIMULATION STUDY OF QUANTUM MECHANICAL CHARGE FIELD (QMCF)*

Wiji Utami

14/373104/PPA/04749

## ABSTRACT

Reactivity of $Ca^{2+}$ ion in liquid ammonia has been investigated using QMCF-MD method. The QMCF-MD method is a framework based on a partitioning scheme which effectively divides the system of study into two regions. The first one contains the chemically interesting species, solvated ion and its first solvation shell, which are treated by quantum mechanics, and the remaining part of the system is treated classically. The aim of this study is to determine the reactivity of $Ca^{2+}$ ion solvation system in liquid ammonia based on radial distribution function, coordination number distribution, angular distribution function, mean residence time and ion-ammonia vibrational frequencies analysis.

*Ab initio* HF/SV(P) and DZP Dunning methods were validated by calculating BSSE energy. The system was equilibrated for 3 ps at 235.15 K, then sampling data was collected every fifth step during simulation time of 12 ps. Result of the study showed that the labile first solvation shell was observed containing of 7-8 ammonia molecules. Mean residence time of ligand in the first solvation shell was 14.45 ps showing few exchanges with second solvation shell. The results show in a good agreement with previous reports both experimental and theoretical studies.

Key words: liquid ammonia, $Ca^{2+}$ ion, Reactivity, MD-QMCF