# A Direct DFT Trajectory Study of the Bis-superoxo $FAl(O_2)_2$ Ionization

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Z. Naturforsch. **63a,** 49 – 52 (2008); received July 3, 2007

Direct density functional theory (DFT) classical trajectory calculations show that after bis-superoxo $FAl(O_2)_2$ ionization, one of the side-on dioxygen units undergoes a fast intramolecular rearrangement generating a stable radical cation which presents both a peroxo and a peroxyl group bound to the central Al atom, $FAl(O_2)OO^{\cdot+}$. Molecular properties of this predicted novel species have been estimated at the B3PW91/6-311+G(3df) and G3B3 levels of theory.

*Key words:* $FAl(O_2)_2$; $FAl(O_2)OO^{\cdot+}$; Classical Trajectory Calculations; Density Functional Theory.