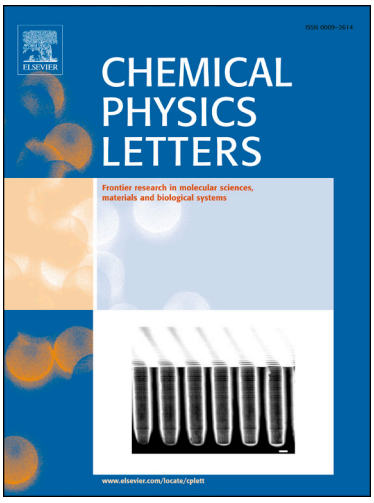


# A practical law to predict the appearance sizes of multiply charged rare-gas and molecular clusters

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# A practical law to predict the appearance sizes of multiply charged rare-gas and molecular clusters

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**Abstract**

A dimensionless law depending on cluster size $N$ is derived from the Rayleigh limit expressed in reduced Lennard-Jones (LJ) units to predict the critical sizes $n_c(z)$ of clusters carrying $z$ positive charges. This relationship provides suitable estimates of $n_c(z)$ ($z = 2-4$) for rare-gas clusters, including neon clusters whose predicted critical sizes deviate from experimental expectations by less than 12% for different choices of LJ parameters. An extension to 11 nonpolar and 15 polar molecular clusters, from dimers to aromatic hydrocarbons, is achieved that demonstrates the broad applicability of the formula despite inaccuracies for highly polar systems.

*Keywords:* Rare-gas clusters, molecular clusters, critical sizes, Lennard-Jones interactions, liquid drop model.

## 1. Introduction

The search for critical (or appearance) sizes $n_c(z)$ above which clusters with $z$ charges are stable is a long-term endeavour. The existence of highly charged metal clusters ($z \leq 14$) has been first observed on sodium clusters by Näher et al. [1]. Although the charge is expected to be distributed over the surface of alkali metal clusters [2], molecular dynamics simulations of uniformly charged sodium clusters following a tight-binding approach [3, 4] yielded $n_c(2) = 27$ and $n_c(3) = 63$ [5], in close agreement with experimental data [1]. However, the critical size obtained for $z = 4$, namely 110, slightly underestimated the experimental values, derived from ion bombardment experiments, that ranged from $122 \pm 2$ ($H^+$ at 5 keV) to $115 \pm 5$ ($^{40}Ar^{8+}$ at 40 keV) [6].

Uniform charge distribution has also been invoked to reproduce the critical sizes of van der Waals and hydrogen-bonded clusters [7]. Clusters are then modeled as continuous media of dielectric constant $\epsilon$ and their total energy is written as the sum of a volume term, a surface term, and a Coulomb term by analogy to liquid drop models (LDMs). Based on the work of Briant and

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