Chemeca2026
Innovate. Integrate. Impact.
28 – 30 September 2026
Melbourne, Australia

Hazards Australasia 2026

Chemeca 2026 and Hazards Australasia
28 – 30 September, Melbourne, Australia

The Impact of Dipole-Dipole Forces on Titania (TiO_2) Nanoparticle Coagulation in the Gas Phase

Xiaoke Wang*

Department of Chemical Engineering, The University of Melbourne, Melbourne, Australia

xiaoke.wang1@student.unimelb.edu.au

ABSTRACT

Titania (TiO_2) nanoparticles (NPs) have received increasing interest due to their excellent optical properties rendering them promising for biomedical applications, such as photothermal therapy (PTT). The structural characteristics of self-assembled NP agglomerates during aerosol synthesis subsequently affect their macroscopic properties. These characteristics are controlled by the van der Waals (vdW) and Coulomb interactions between NPs. However, existing theories (e.g., Hamaker theory) quantifying the interactions between NPs in the gas phase overlook the role of Coulomb forces, even though the latter can exceed the strength of the vdW interactions. Despite this, the effect of the orientation of NP dipole moments on overall interparticle interactions is still poorly understood.

Here, the potential of mean force (PMF) between evenly-sized 2 – 8 nm bare and hydroxylated TiO_2 NPs is obtained by molecular dynamics (MD) simulations. The NPs relative dipole moment orientations affect the magnitude of the overall NP-NP interactions, with "tail-to-tail" alignments leading to repulsive interactions and "head-to-tail" arrangements resulting in attractive forces (Figure 1a: insets). Interparticle dipole-dipole interactions are mainly controlled by the "head-to-tail" dipole-dipole configurations corresponding to the lower boundary of the PMF (minimum PMF, Figure 1a).

Figure 1b shows the minimum PMF between two 2 – 8 nm TiO_2 NPs at point contact ($d_s = 0$) as a function of the dipole moment, p, at 500 K for different OH coverages. The PMF is calculated over 1000 relative dipole moment orientations (shaded area in Fig. 1a). Insets represent the schematic diagrams of TiO_2 NPs at low (4.8 OH/nm^2) and full OH surface coverages (14.6 OH/nm^2). The strength of the interparticle attractive interactions increases with increasing dipole moment, p, which is controlled by tuning the NP OH surface coverage. Figure 1b also compares the results with the Hamaker theory (dot with error bars), which significantly underestimates the interaction energy by up to 84% even for bare TiO_2 NPs. The obtained PMF profile can be employed into mesoscale simulations for accurate prediction of NP coagulation in the gas phase.

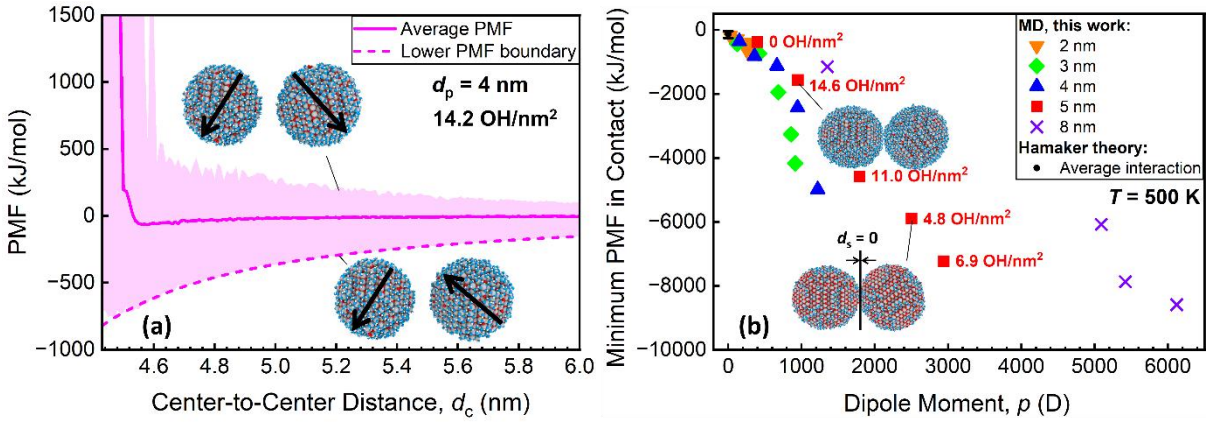

Figure 1. (a) PMF between two fully hydroxylated TiO_2 NPs as a function of the particle centre-to-centre distance, d_c, at 500 K. (b) Minimum PMF at d_s = 0 between two 2 – 8 nm rutile TiO_2 NPs as a function of the dipole moment, p, at 500 K, obtained by MD (filled symbols) and by the Hamaker theory with $A_H = 2.87 \times 10^{-19}$ J. Insets show the configuration of low and full OH coverages.

KEY WORDS

Nanoparticle interactions, dipole moment, molecular dynamics, photothermal therapy

BIOGRAPHY

Xiaoke Wang is currently a PhD candidate at The University of Melbourne, Melbourne, Australia. Her research focuses on the fundamental theory of fractal-like nanoparticles on cancer treatment using multiscale simulations of titania (TiO_2) nanoparticles in the gas-phase by molecular dynamics (MD). In addition, she is also interested in exploring the reaction mechanisms of titanium tetra-isopropoxide (TTIP) in flames using density functional theory (DFT) and statistical reaction rate theory.

CONFERENCE PROGRAM

Please indicate which conference program your abstract relates to:

☐ Hazards Australasia

☒ Chemeca