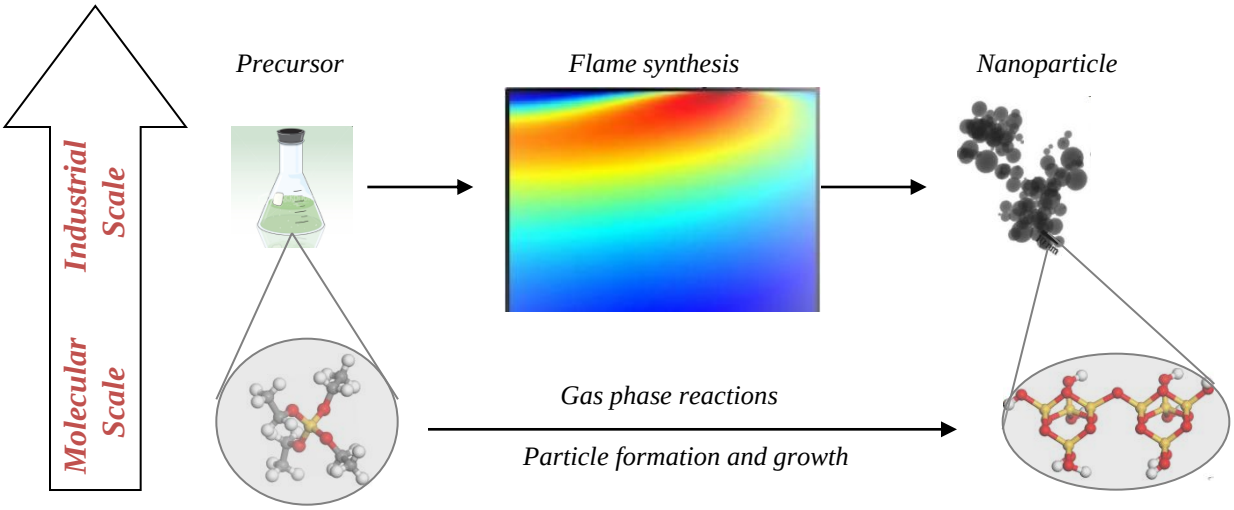
user story

# *Ab initio* modelling of nanoparticle systems

## Understanding particle synthesis routes to determine product properties




Nanoparticles find widespread applications in numerous fields ranging from catalysis to sunscreens to biotechnology. It has been demonstrated that the rates of gas phase reactions which lead to particle formation are important in determining the final product properties, and thus a detailed knowledge of these processes is essential.

### THE CHALLENGE

Understanding mechanisms of nanoparticle synthesis.

### THE SOLUTION

Coupling a kinetic model developed from first principles (using Quantum mechanics and Statistical thermodynamics) with a detailed population balance model to simulate an industrial scale reactor.

### THE RESULTS

- Molecular level calculations and thermochemistry of all chemical species involved in the system.

- Kinetic model generated using thermochemistry information and optimisation techniques.

- Kinetic coupled to a stochastic population balance solver to produce a detailed overall model.

Silica nanoparticles have been adopted in a diverse range of industrial applications. The structure of silica make it useful as a substrate for active substances such as expensive metals and polymers. The formation of silica nanoparticles from tetraethoxysilane (TEOS) using thermal decomposition methods such as flame spray pyrolysis (FSP) is one of the most popular routes for the synthesis of these particles. Despite its industrial importance, the current knowledge of gas-phase decomposition of TEOS to eventually form silica particles remains incomplete.

### THE CHALLENGE

In order to control the final particle size and morphology, we require a comprehensive understanding of the nanoparticle synthesis route on a molecular level. *Ab initio* modelling tracks the evolution of a chemical system from the molecular level to the industrial scale. Our work demonstrates the feasibility of using first-principles modelling to understand complex nanoparticle systems of industrial import.

### THE SOLUTION

First principles modelling of a system involves the following steps: firstly, quantum chemistry calculations are used to determine system properties on a molecular level. This information is scaled to a macroscopic level using statistical thermodynamics. This thermochemistry is then used to generate a kinetic model which when coupled to a detailed population balance model generates the overall model.

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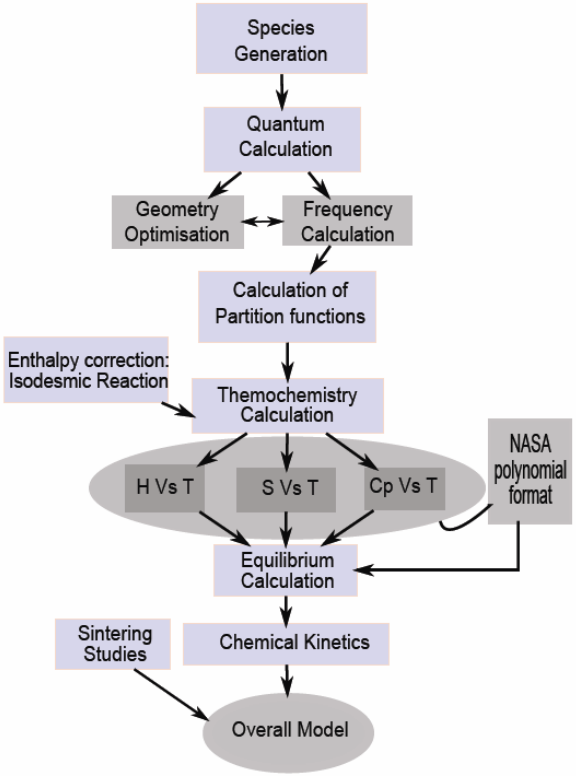
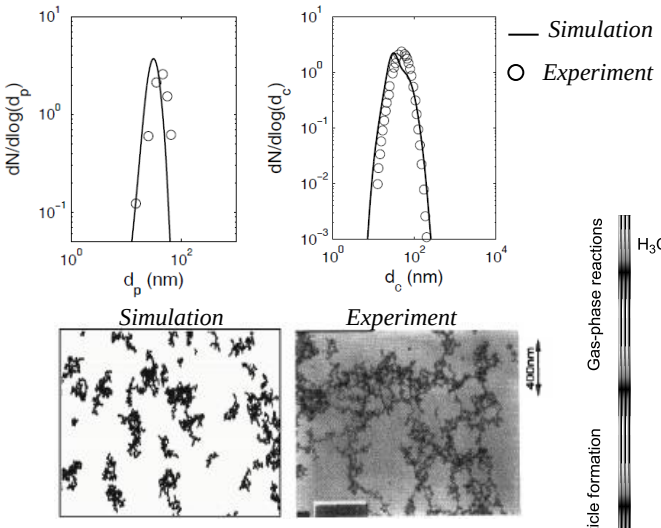



Steps involved in modelling a nanoparticle system using first principles.




Final silica nanoparticle size distribution and TEM images. Experimental values are from Seto *et. al.*
doi:10.1080/02786829708965482

## APPLICATION AREAS

•Nanoparticle systems using gas phase synthesis methods.

## PRODUCTS USED

- Quantum Chemistry Solver
- Gas-phase chemistry solver
- Stochastic population balance solver

## THE RESULTS

### • Quantum Chemistry and Statistical thermodyamics

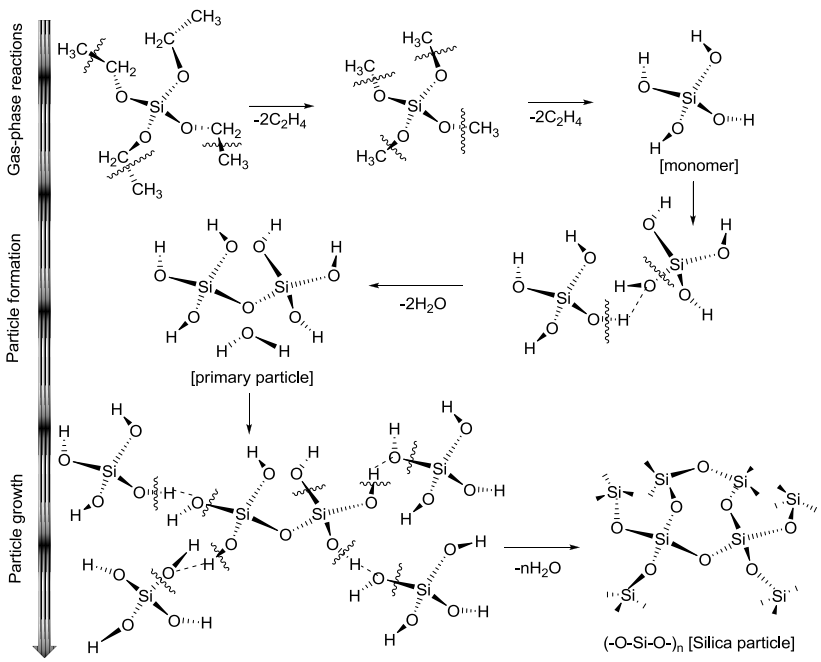
The optimised geometries and frequencies of all the species likely to exist in the reaction system are first determined by solving the time invariant Schrödinger equation. These frequencies are then used to calculate the partition functions using statistical mechanics to determine the thermodynamic and transport properties of the system on a macroscopic level.

### • Kinetic Model

The thermochemistry of the system is used to obtain the equilibrium composition of the system, which can then be used to systematically generate a reaction mechanism. The rate parameters of the kinetic model are fitted to experimental data using sophisticated optimisation techniques.

### • Population Balance Model

A multi-dimensional stochastic population balance model is used to describe inception, surface growth, coagulation and sintering of particles. The kinetic model is then coupled with the population balance model using an operator splitting technique to generate the final overall model.




Silica nanoparticle synthesis route determined using first principles The precursor decomposes to form gas phase monomers which undergo dehydration to generate web like silica nanoparticle

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