

Debora Monego^{1,2}, Stefano Bernardi^{1,2}, Paul Mulvaney^{1,3}, Asaph Widmer-Cooper^{1,2} ¹ARC Exciton Science, ²University of Syndey, ³University of Melbourne x10⁹ s.m **Our approach** Analytical **Ultracentrifigation (AUC)** Cloroform nanocrysta solvent solution reference blank) CdSe nanoparticles **Stokes-Einstein-Sutherland** (SES) Equation -SC₁₈ ligands $6\pi\eta R_{\rm sh} + 6\pi\eta R_{\rm c}$ $k_{\rm b}T$ $k_{\rm b}T$ DFor SES to be valid for our nanocrystal solution, two conditions must be met: Compression Bundle Shell thickness (R_{sh}) is constant **AUC experiments +** Interdigitation **Molecular dynamics simulations** No-slip boundaries **2** 2400 4.0 nm 2.5 3.0 3.5 Core surface spacing s 2200 2000 **Our hypothesis:** Ligand shell thickness changes with particle size 1800 Defining shell thickness using the 1600 sit g/cm³ **Gibbs dividing surface:** The second secon 6 nm 4 nm **ŏ** 1400 **Gibbs dividing No-slip condition is met for** surface 1200 0 our systems! ≥1. 1000 average density Slip length 、 inside ligand shelf 800 ligand ____

SYDNEY SYDNEY SYDNEY SYDNEY **Characterising apolar nanocrystals is difficult** dominated 80 100 120 140





Key results:

in our particles.

2. A shell thickness that changes with core size should be considered when calculating their hydrodynamic radius from AUC data.

Characterising colloidal nanoparticles with small cores is possible with AUC as long as the experiments are carried out in combination with simulations that provide a self-consistent estimate of the shell thickness and density for the given system



Considering the ligand shell thickness to be 1.78 nm or the maximum extent of the ligands does not yield good agreement between AUC experiments and MD simulations.

Conclusions

1. No-slip condition is met for ligand/solvent interface

Broader implications: