

Designing Nanocrystal Surfaces for Accessing Metamaterials



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Basic Energy Science

<https://youtu.be/Vb3qnG68XX8>

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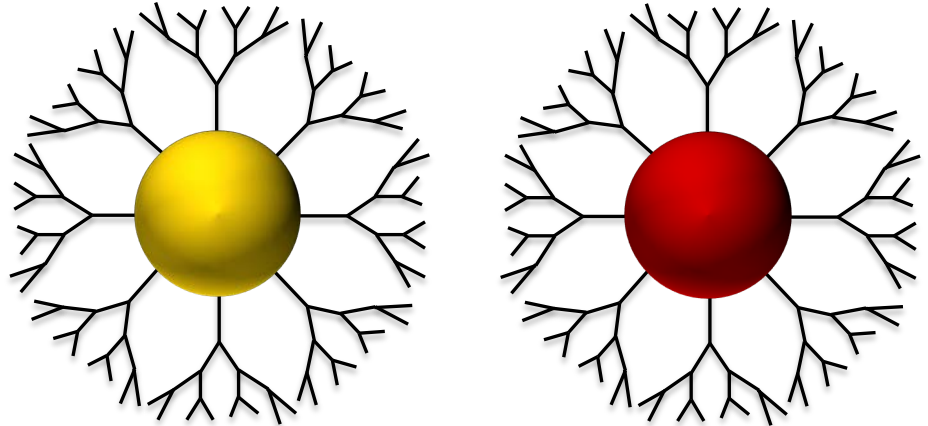
Introduction

- We think about nanocrystals as building blocks to create materials with unique or advanced properties and applications
- Our material's properties come from a combination of the nanocrystal itself, ligands on the nanocrystal surfaces, and how the nanocrystals are arranged in thin films
- Studying coordination and self-assembly behavior of ligands on nanocrystals for understanding and engineering various properties
- Majority of current research conducted with commercially available ligands
- Design of novel ligands can lead to more targeted function
- A major challenge in accessing metamaterials or advanced materials is phase segregation of the component nanocrystals



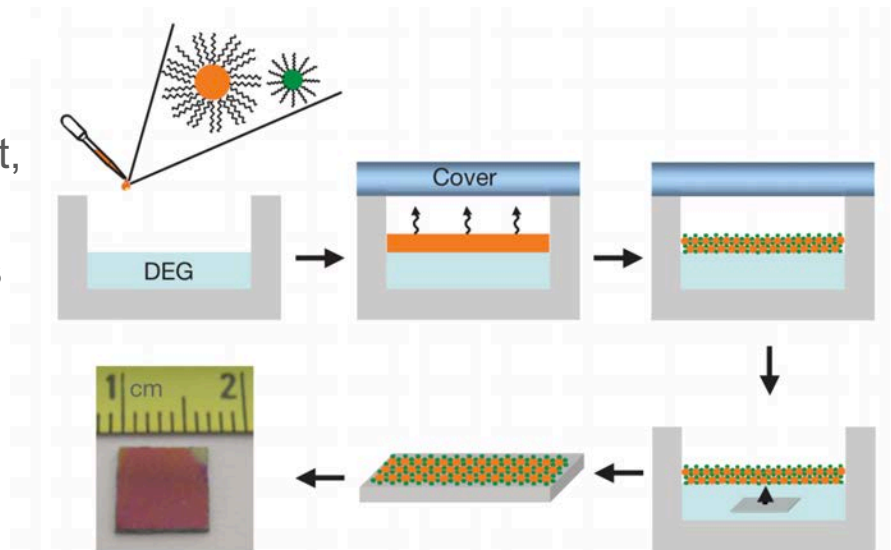
Objective

- Design and make our own surface ligands for nanocrystals that target specific properties
- Focus on incorporation of two distinctly different nanocrystals into one thin film
- Ultimate goal of rationally designing materials for their properties, without limits of complimentary nanocrystal size, shape, or composition
- This goal allows for access to materials with applications in catalysis, renewable energy generation and storage, and optics

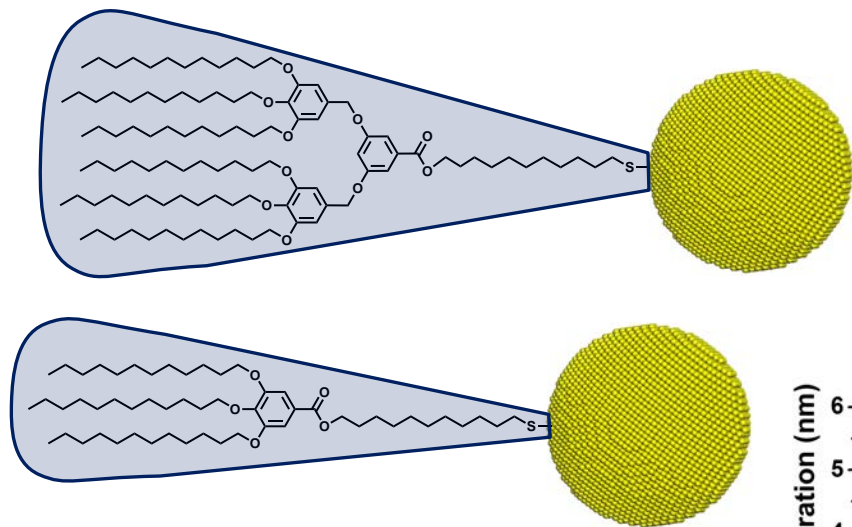


Methods

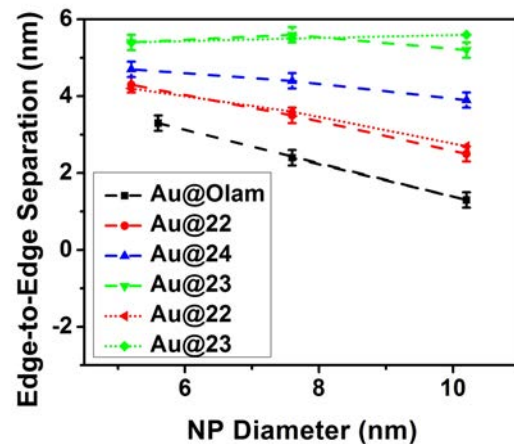
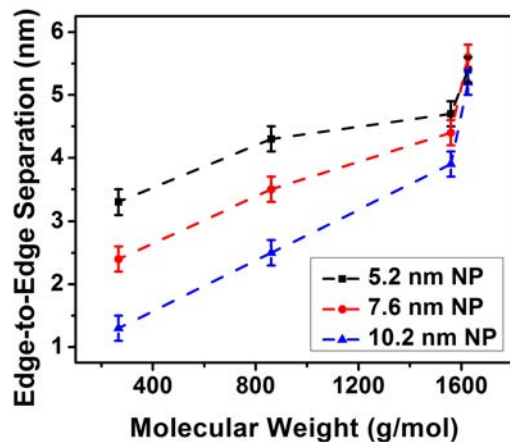
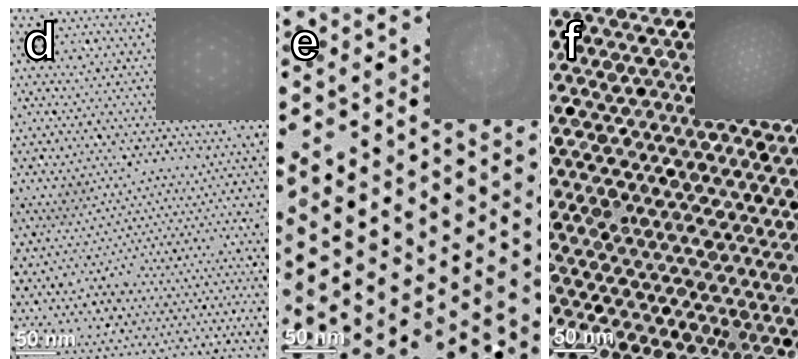
- Design and synthesize surface ligands
- Separately, synthesize nanocrystals
- Graft newly synthesized ligands onto the nanocrystal surfaces
- Assemble nanocrystals into thin films
- Build knowledge of spherical systems first, then expand to other nanocrystal shapes and compositions to develop design rules



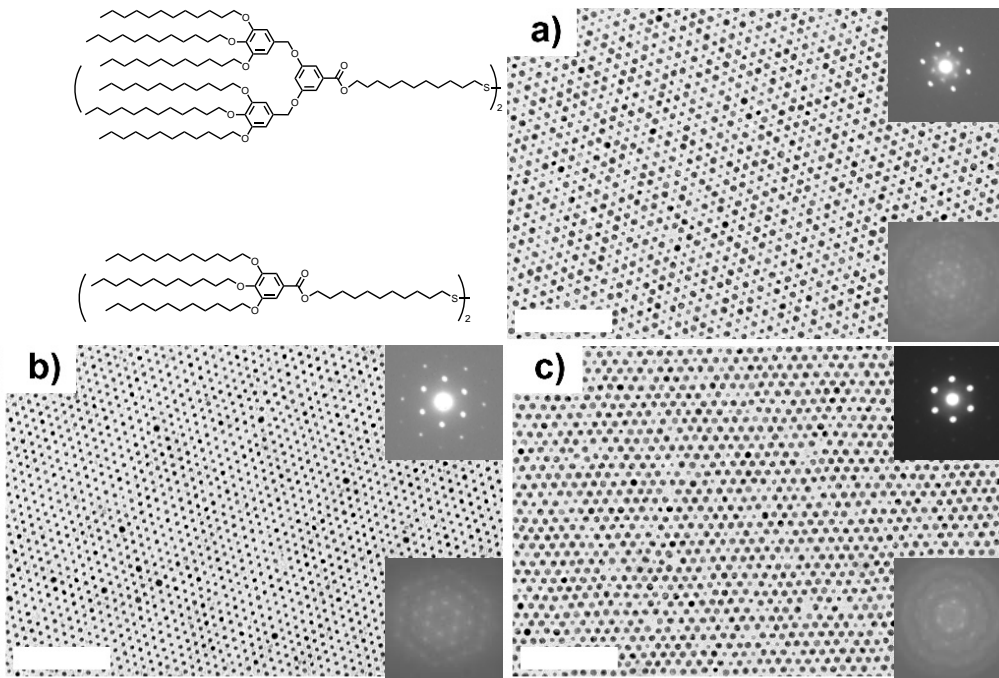
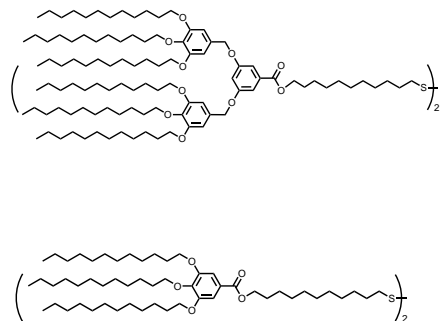
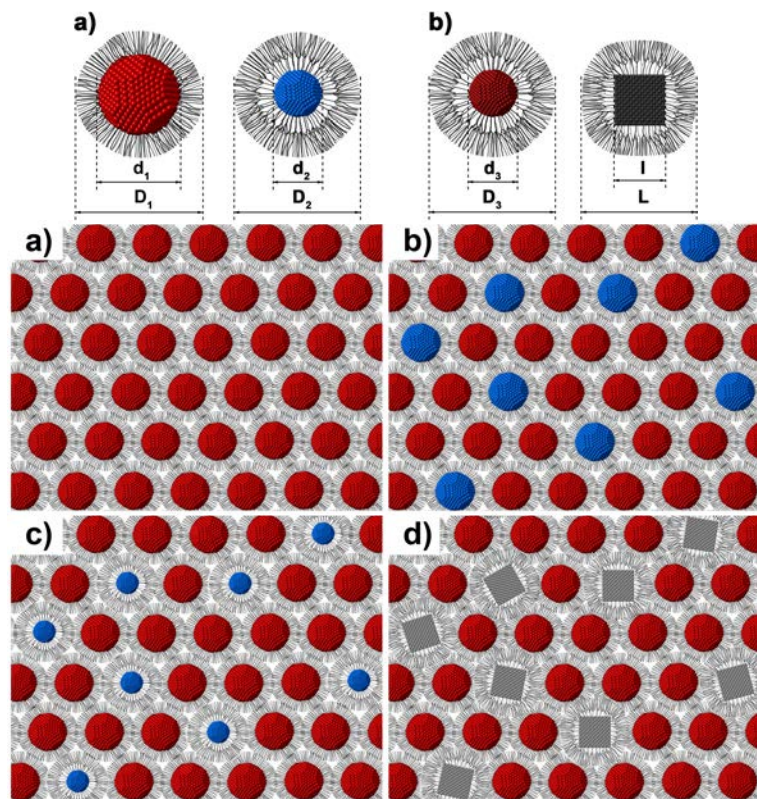
Promising Results Maintaining Interparticle Spacing



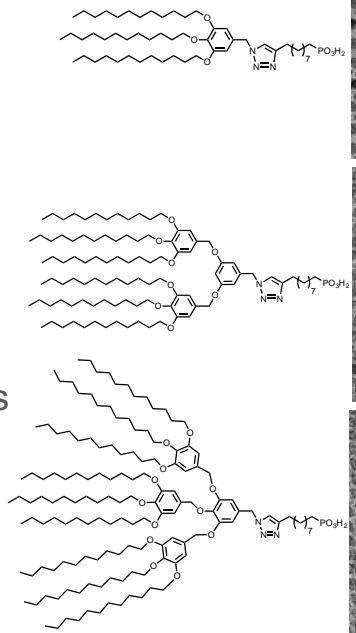
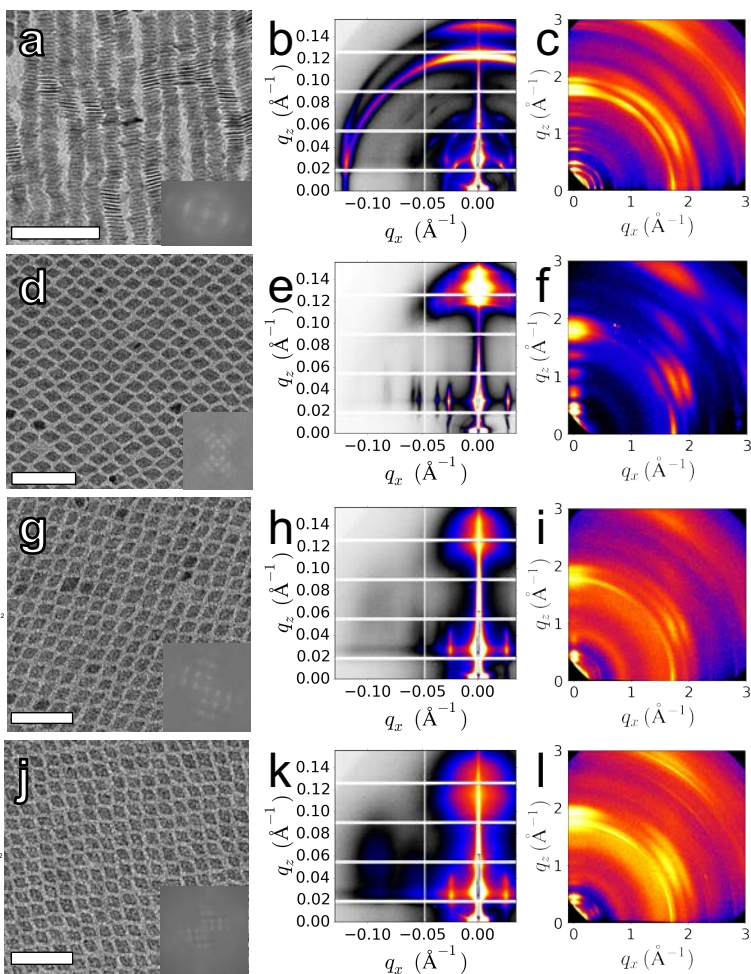
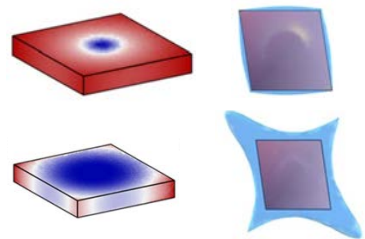
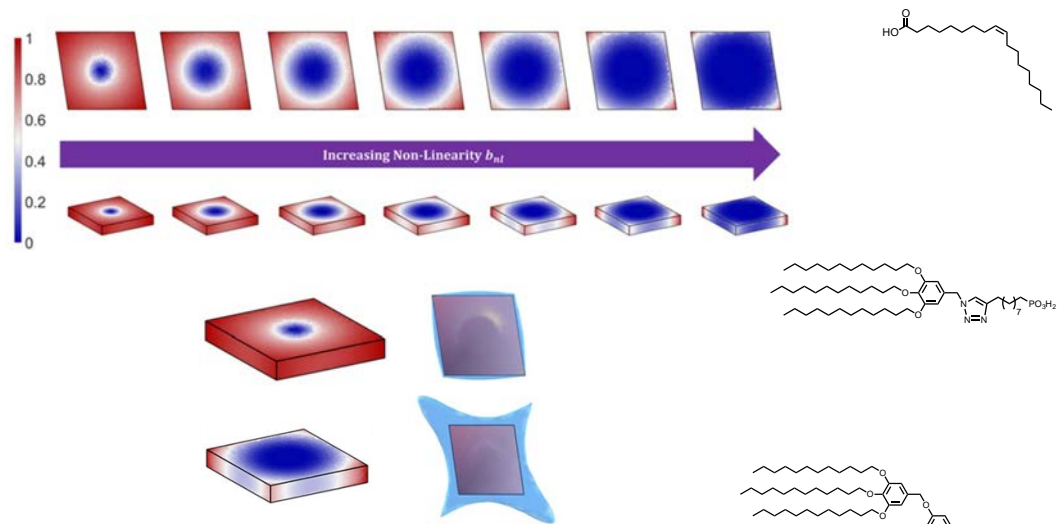
- Dendrimers are able to maintain constant distances in between NCs of differing sizes
- This effect is mainly due to the dense packing of the ligands, as cones can fit tightly around spheres



Utilizing the Ligand Shell to Enable Nanocrystal Mixtures

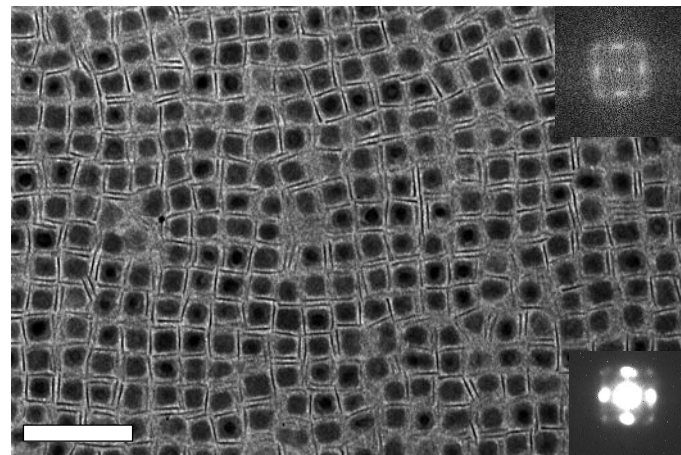
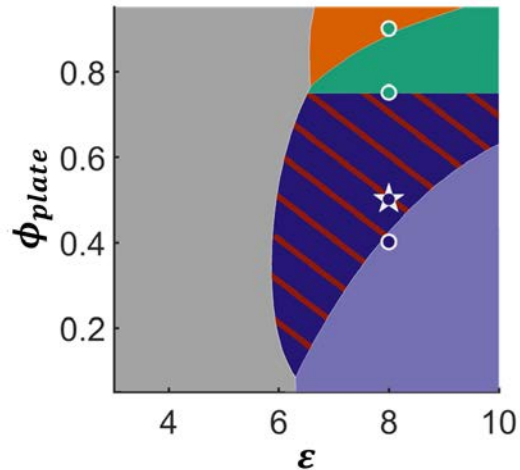
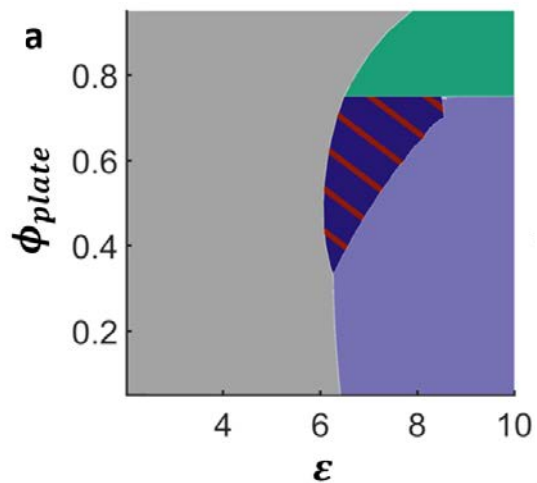
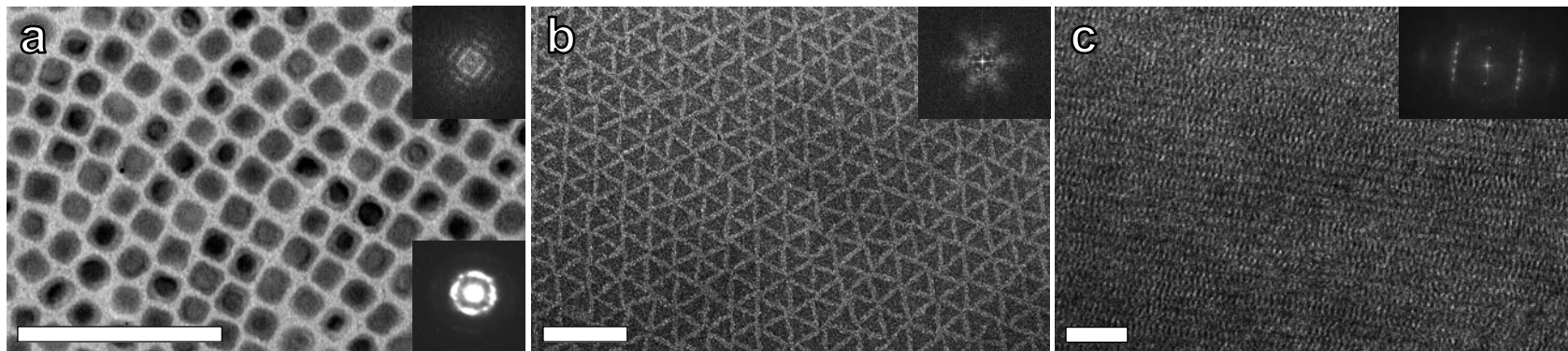


What if the Nanocrystal is not a Sphere?



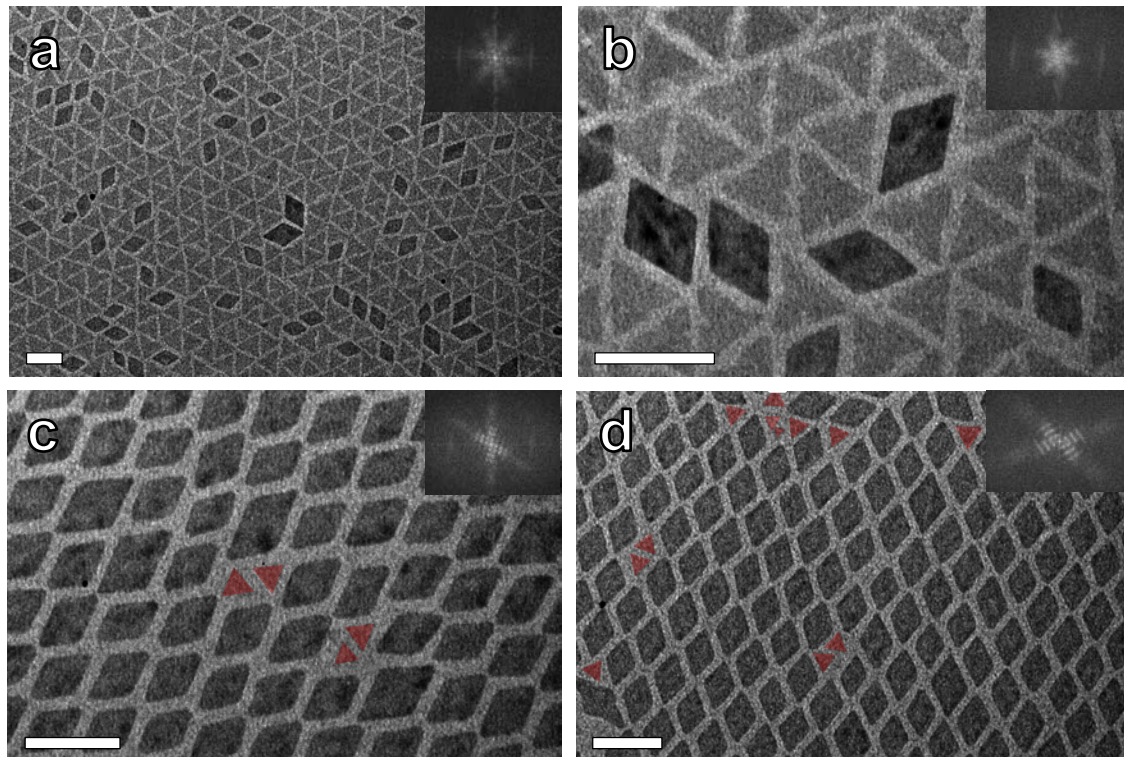
- Ligands with higher branching preferentially bind to the corners and edges of these plates, creating a non-uniform corona around the NCs
- This non-uniform corona can be used to guide NC arrangements in thin films

Rational Design of Anisotropic Nanocrystal Assembly



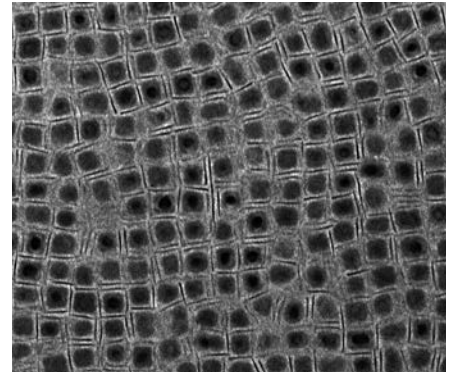
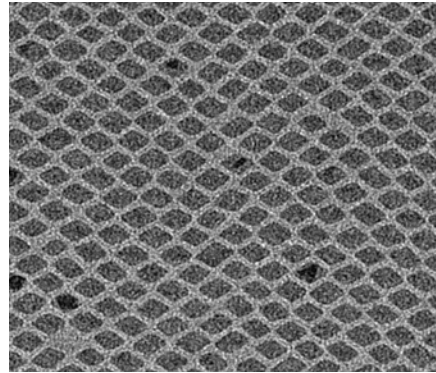
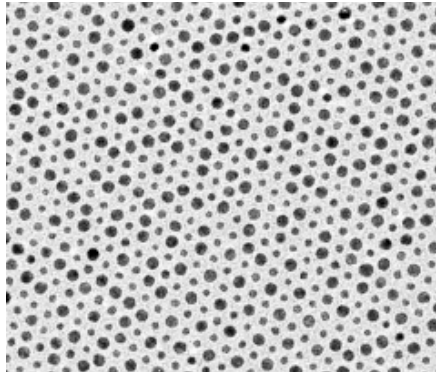
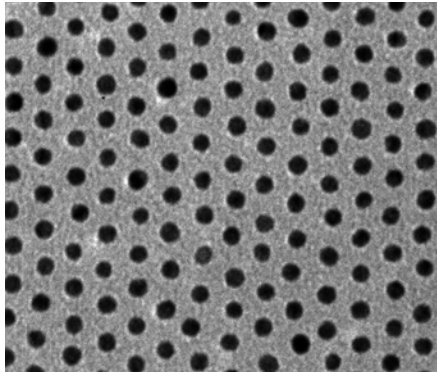
Rational Design of Anisotropic Nanocrystal Assembly

- Applying the design rules we have learned across multiple materials choices
- Maintain crystallinity of the thin film while incorporating different materials
- Change component ratios based on researcher's goals



Conclusions

- Ligand choices for building knowledge for design rules
- Intentional design for targeted assembly
- Fundamental studies towards metamaterials and advanced materials efforts



Future work

- Now that we understand how we can modify the surfaces of nanocrystals to effectively create thin films made of distinct types of nanocrystals, we can take the next step and choose our nanocrystal building blocks to target specific properties
- Expand our experimental knowledge further to enable inverse design of metamaterials
- This work provides a fundamental basis for the development of metamaterials that can be used in a variety of applications

Acknowledgments

