2d colloidal nanocrystal for optoelectronic and solar cell

Novel 2D colloidal nanocrystal for optoelectronic and solar cell applications

Recently, 2D material has attracted tremendous attention due to their fascinating physicochemical properties. Particularly, the discovery of graphene, a single layer of carbon atoms arranged in a 2D honeycomb lattice has ignited the research on this class of 2D materials due to extraordinary mechanical, electric and optical properties not observed in their bulk counterparts. Considering graphene is a simple material composed of only carbon element, it cannot satisfy the increasing requirements of diverse applications due to limitations in the versatility and the tunability of composition, structure and functionality in addition to the paradox between the high-mobility Fermi−Dirac electronic structure and the need for a size-dependent band gap for traditional semiconductor devices. As a result, of paramount importance and interest is to search alternative 2D materials which possess much more flexibility and diversity of composition, structure, and functionality. Layered metal dichalcogenides such as WS2 and MoS2 have been extensively investigated. Like graphite, the atoms within the host layers form strong covalent bonding with relatively weaker interactions between layers such as van der Waals force. Consequently, micromechanical cleavage by Scotch-tape is the most straightforward method to obtain an individual layer while retaining their intrinsic host structure. Though it is crucial to evaluate their physical properties, this approach is time-consuming and the yield is also low. More recently, a direct liquid exfoliation where a suitable solvent is selected to stabilize cleaved crystallites was proposed to produce nanosheets. This process, comprised of ion-exchange, osmotic swelling, and exfoliation, is useful, but the concentration of unilamellar

nanosheet in the solution is still very low with the yield no more than a few tens of percentage and the properties of the resulting nanosheets are dictated by their parent 3D materials, which loses the opportunities to design and control over chemical composition and structure. In order to meet the demand for fabrication of functional nanostructured electronic and optoelectronic devices, a facile process to produce large amount of 2D nanocrystal (NC) with possibility of tuning the properties is really imperative.

Colloidal chemical synthetic route has been demonstrated highly attractive and powerful for their low-cost synthesis to obtain NCs from solution in excellent yield with a good uniformity in terms of chemical composition, surface properties, shape, and size. The complete control over size, shape and structure of the colloidal NCs via tuning reaction chemistry provides new pathways to design material where size or shape dependent properties can be exploited. *In this project, the metal dichalcogenides such as MoS2 and WS2, typically with a trilayer structure of covalently interconnected layers of S, M, and S atoms, will be the main candidates. High performance solar cells built from them in 2D NC form is the final goal. As such, colloidal synthetic route will require balance of the reagent choice and reaction chemistry to accurately control the growth in the NC.*

All the advantages of 2D colloidal NCs will be exploited to fabricate solar cells in low cost while retaining efficiencies towards 10%. The objectives of this proposal are as follows:

1. Develop colloidal synthetic routes for 2D colloidal NCs.

2. Balance the reagent choice and ligand chemistry to achieve NC growth with controllable size, shape, and particularly thickness.
3. Assemble 2D colloidal NCs to device scale area and perform correlative material studies with electronic properties (carrier lifetime, photoluminescence, carrier mobility).
4. Fabricate all-inorganic NC solar cells and optimize in the device parameter space towards high power conversion efficiency.

The project will be divided into three work packages (WPs) with a number of tasks in each WP structured to achieve the aims and objectives.

Work Package 1 Controllable synthesis

Task 1. 1Develop colloidal synthetic routes to 2D semiconductor NCs.

Hot-injection method which involves the injection of a cold solution of precursor molecules into hot liquid will be employed due to the instantaneous formation of nuclei with slow growth of the existing nuclei but not to new nucleation for well controlled size and thickness. The product will be separated by centrifuging and washed up for characterization and analysis by XRD, electron diffraction and HRTEM for structure, and EDS and Raman for chemical composition.

Task 1. 2Monitor and control the thickness, doping and their effect on the optical properties.

Unlike 0D and 1D NC, in addition to control over composition and structure of 2D NCs, of particular interest is to rationally design and tune the thickness-dependent optical and electronic properties. For example, few-layer MoS2

has an indirect bandgap, but when it is thinned to single-layer, it becomes direct bandgap leading to enhanced photoluminesence. In this task we will monitor the effects of the thickness distribution particularly on absorption and photoluminescence (lifetime and QY). The latter will also be used as a metric to decide on the more promising routes for device fabrication, focusing on highly PL materials as the most promising candidates. In addition, substitutional or interstitial doping of metal sites within 2D NC may be employed to engineer optical characteristics.

Work Package 2 Optoelectronic Properties of NC solids

The presence of covalently bound ligands on the surface of colloidal NC provide a versatile synthetic handle for tailoring the structure, stability, and importantly electronic and optical properties. The deviation of composition and atom arrangement along the terminating edge and corner sites of 2D colloidal NCs also offers another way to tune their properties. One of the key determinant factors of the performance of solar cells is the carrier mobility. In this task we will investigate ligand exchange strategies using ligands that are shorter than 0. 3 nm and contain functional head groups such as di-thiol groups and carboxyl-acid based groups. At the same time those functional groups should serve to passivate dangling bonds and therefore their electron-donating density will be chosen accordingly. We will monitor the effect of those ligands on carrier mobility by performing CELIV measurements in diode structures resembling an actual solar cell device architecture as well as using FET mobility measurements.

In addition to high carrier mobilities NC solids for efficient solar cells call for long carrier lifetimes. Such long lifetimes can be achieved by suppressing trap states and recombination centers typically caused at grain boundaries and interfaces. The role of this task is to monitor the degree of passivation of the ligands utilized with Photoluminescence and PL-lifetime measurements.

Work Package 3 Photovoltaic device fabrication, testing and optimizing

Task 3. 1We will develop simple Schottky and bilayer heterostructures in which the sole photoactive layer is the 2D NC which can be achieved by using a transparent n-type high bandgap semiconductor to form a junction. We will then perform carrier lifetime and recombination-rate characterization employing transient photovoltage and photocurrent measurements.

Task 3. 2Optimization of heterojunctions based on 2D NCs.

We will perform a device optimization study in which we will study the effect of layer thickness and contact selection to maximize efficiency. The optimized thickness will be sought as a combination of the expected carrier diffusion length and achievable depletion widths based on the mobility, lifetime and carrier density of the semiconductor. Appropriate contacts will be investigated based either on inorganic (MoOx) or organic hole transport layers (electron blocking layers).