Computational and Experimental Studies for Advancement of Electronics, Oil and Gas, and Solar Energy Systems

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A safe and secure future for humanity depends to a large extent on the development of sustainable and economic energy resources, and will require fundamental science and engineering contributions. In this talk I will present some of my work on the advancement of energy systems in electronics, oil and gas, and solar energy sectors.

Cooling of electronic systems, particularly high performance data centers, is a highly energy intensive process. In 2013, data centers consumed about 100 billion kWh of electricity in the U.S. alone and it is expected that by 2020, the carbon footprint of data centers will exceed that of the airline industry. One of the solutions to reduce energy consumption is to move from conventional air cooling to liquid cooling, and in that respect I will present a computer-aided molecular design approach for development of novel heat transfer fluids for cooling of such systems. The fluids designed in this work not only possess superior heat transfer properties, but also significantly lower global warming potentials. I will also present a critical evaluation of nanoparticle dispersions (or nanofluids) for heat transfer applications and show, contrary to widely held belief, the effective thermal conductivity of nanofluids decreases with decreasing particle size.

In conventional oil and gas industries, clathrate hydrates of natural gases are associated with many energy transportation (‘flow assurance’) related problems. However, gas hydrates also present a potential future energy resource, as it is estimated that more than 10^{15} m^3 of natural gas is present in oceanic and permafrost gas hydrate deposits. I will present some of my work on hydrate phase equilibria modeling, including the application of a quantum chemical approach, COSMO, and flowloop studies carried out at the Exxon-Mobil flowloop facility.

I will also present my work related to the solar industry, which has been growing at a tremendous pace for the last 10-15 years. As the price of solar grade silicon has dropped from about $350/kg in 2008 to about $19/kg in 2015, there is a considerable need to advance and optimize process systems in the solar industry. I will present a few examples from manufacturing of silicon for photovoltaic applications, and how a lack of thermophysical property data on chlorosilanes and poor assumptions in process design affect the productivity of silicon.