The Hong Kong University of Science and Technology

Department of Mathematics

<u>Seminar on Applied Mathematics</u>

Revisiting surface elasticity theory from an orbital-free density functional theory perspective

by

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<u>Abstract</u>

In this presentation, the well-established Gurtin-Murdoch theory of surface elasticity (Gurtin and Murdoch, 1975, 1978) is revisited from an orbital-free density functional theory (OFDFT) perspective by taking the boundary layer into consideration. Our analysis indicates that firstly, the quantities introduced in the Gurtin-Murdoch theory of surface elasticity can all find their explicit expressions in the derived OFDFT-based theoretical model. Secondly, the derived expression for surface energy density captures a competition between the surface normal derivatives of the electron density and the electrostatic potential, which well rationalises the onset of signed elastic constants that are observed both experimentally and computationally. Thirdly, the established model naturally yields an inversely linear relationship between the materials surface stiffness and its size, which conforms to relevant findings in literature. Since the proposed OFDFT-based model is established under arbitrarily imposed boundary condition of electron density, electrostatic potential and external load, it also has the potential of being used to investigate the electro-mechanical behaviour of nanoscale materials manifesting surface effect.

Date: **Thursday, 14 February 2019**
Time: **3:00p.m. – 4:00p.m.**
Venue: **Room 3472, Academic Building, (Lifts 25-26), HKUST**

All are welcome!