



**The Hong Kong University of Science and Technology**

**Department of Mathematics**

**Seminar on Applied Mathematics**

**The missing gene for ferroic material design: phase transition graph**

*by*

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**Abstract**

The symmetry of a crystal has profound effects on its physical properties and so does symmetry-breaking on the characteristics and properties of a structural phase transition. For an important class of smart materials, the ferroics, their functionality and performance are associated with cycling transitions from multiple structural states of one phase to those of the other, for which existing theories do not apply. Using group and graph theories, we construct phase transition graph (PTG) and show that both the functionality and performance of ferroics are dictated by the topology of their PTGs. In particular, we demonstrate how giant piezoelectricity in ferroelectrics and functional fatigue in shape memory alloys (SMAs) are related to their unique PTG topological features. Using PTG topology as a generic guide, we evaluate systematically new systems potentially having giant piezoelectricity and giant electro- and magnetostrictions and discuss design strategies for high performance SMAs with much improved functional fatigue resistance [Acta Mater. 127 (2017) 438-449].

**Date: Thursday, 12 April 2018**

**Time: 3:00p.m. – 4:00p.m.**

**Venue: Room 2408, Academic Building  
(near Lifts 17 & 18), HKUST**

***All are welcome!***