



Solid State Institute  
המכון למצב מוצק

TECHNION  
Israel Institute  
of Technology



הטכניון  
מכון טכנולוגי  
לישראל

SPECIAL SEMINAR

סמינר מיוחד

## “Understanding materials from first-principles calculations”

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Chancellor

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### Abstract

With the rapid advancements in modern computational techniques, computational studies of condensed matter have become increasingly important in understanding physical mechanisms, simulating dynamical processes, and designing desirable materials. In this talk, I will use new solar energy materials as examples how first-principles calculations can be used to comprehend their unique properties. Specifically, I will discuss the defect properties of semiconductors and how illumination affects the properties of carriers in these materials. In addition, I will present systematic results on the stability of perovskite  $ABX_3$  materials, which have been experimentally proven to be highly efficient solar energy materials. Finally, I will briefly discuss some remaining key challenges in this field and how artificial intelligence can provide novel opportunities for first-principles calculations.

Prof. Xin-Gao Gong received his Ph.D from the Institute of Solid State Physics, Chinese Academy of Sciences in 1993, since then he became a full professor in the same institute. He joined the Fudan university in 2000 and is currently a Xie XiDe Chair Professor of Physics, and also Director of Key Laboratory of Computational Physical Sciences, Ministry of Education. His research is focused on the computational studies of structural and electronic properties of materials. He is a fellow of the American Physical society, and Academician of Chinese Academy of Sciences. Since 2021 he has been the Chancellor of Guangdong Technion-Israel Institute of Technology.



ההרצאה תתקיים ביום רביעי, ה-24.5.23 בשעה 14:30  
באודיטוריום המכון למצב מוצק, קומת כניסה

The lecture will take place on Wednesday, 24.5.23 at 14:30  
at the Solid-State Institute auditorium, entrance floor

Refreshments (“Pizzot”) at 14:15

כיבוד ("פיצות") בשעה 14:15

Host: Professor Oren Cohen and Professor David Gershoni