**Dr. Ching-Ming Wei**

Distinguished Research Fellow,

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Honors and Awards:

1994 Outstanding Research Award, National Science Council, Taiwan

1996 Achievement in Asia Award, Oversea Chinese Physics Association (OCPA)

1997 Fellow, Taiwan (ROC) Physical Society, Taiwan

1999 Outstanding Research Award, National Science Council, Taiwan

2004 Outstanding Research Award, Ministry of Science and Technology, Taiwan

2011 Fellow, American Physical Society (APS)

2020 Outstanding Special Researcher Award, Ministry of Science and Technology, Taiwan

**Time：**2022/01/25 11:00-12:00

**Location：****Jhongjhe**ng Hall中正堂

**Title：**Computational Materials Studies Using DFT and DQMC

Computational Materials Studies Using DFT and DQMC

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I will discuss computational materials studies using density function theory (DFT) and diffusing quantum Monte-Carlo (DQMC). Using DFT, we have found the quantum size effect (QSE) in metallic thin films can be correlated with the thickness dependence of the energies of confined electrons. The oscillations, in surface energy, work function, and superconducting temperature, as a function of film thickness can be well fitted by damped sinusoidal functions with their periodicity determined by one Fermi wave vector or a combination of several Fermi wave vectors along the thin film’s direction. A quantitative description of these QSE requires the full consideration of the crystal band structure. Using DQMC, we studied the adsorptions of CO molecule on various fcc(111) surfaces (Rh, Ir, Pt, and Cu) and have found that the top site is the most stable adsorption site in agreement with experiments. Compared to the DQMC results, DFT calculations with the generalized-gradient approximation (GGA) predict very similar adsorption energies on the top site, but they overestimate those on the bridge and hollow sites. These results explain why the top site adsorption for CO on Rh, Pt, and Cu(111) surfaces was not predicted correctly by the previous standard local or semi-local DFT calculations. In the final part, I will discuss the Sb, Bi doping, and Ge vacancy dependence of the lattice thermal conductivity (κL) in GeTe by solving the linearized Boltzmann equation based on first-principles anharmonic lattice dynamics calculations. To tackle the numerical complexities of third-order force constants, we used machine learning methods to the construct force constant models. We have found a dramatic reduction of κL in GeTe doping solutions and in Ge-vacancy systems due to the lowering of the phonon lifetime. Our findings indicate an optimum dopant percentage of 3-5% to boost GeTe thermoelectric temperature efficiency and have provided a benchmark for understanding the origin of high figure of merit (ZT) in GeTe related materials.