# 物理博一許誌恩 連續發表論文登英美國際期刊

學習新視界

【記者麥嘉儀淡水校園報導】物理系教授薛宏中、助理教授李啟正及理學院應用科學博一許誌恩，共同發表論文「新的原子震盪計算方法：以鹽與鉛鈦氧化薄層的原子為例」（Partitioning interatomic force constants for first-principles phonon calculations:Applications to NaCl, PbTiO3, monolayer CrI3, and twisted bilayer graphene），刊登於英國物理學會期刊「 Journal of Physics: Condensed Matter」，其影響係數為2.745（2021）。

他最新投稿一篇論文題目：「硫化錫晶體中向列的電子與聲子動力學」（Nematic electron and phonon dynamics in SnS crystals ），也成功被美國物理聯合會「Applied Physics Letters」接受，其影響係數為3.971，即將刊登。

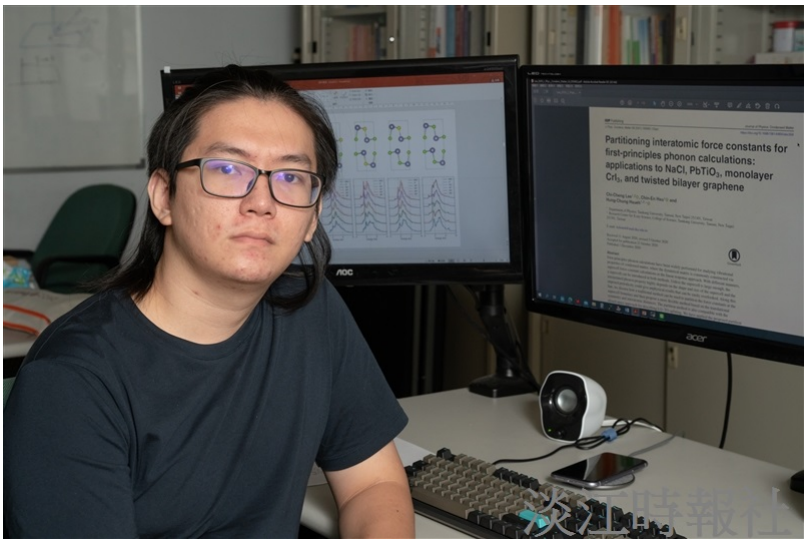
本學期剛從碩一直升博一的許誌恩，原本英文程度就不錯，大一念彰化師大數學系，大二轉入本校物理系，發現自己的研究興趣，大三升大四時完成此篇論文投稿，他在大學時即修習研究所課程，為專心做研究，已經把博士班課程修完了，被物理系主任莊程豪喻為學術研究的「新星」。

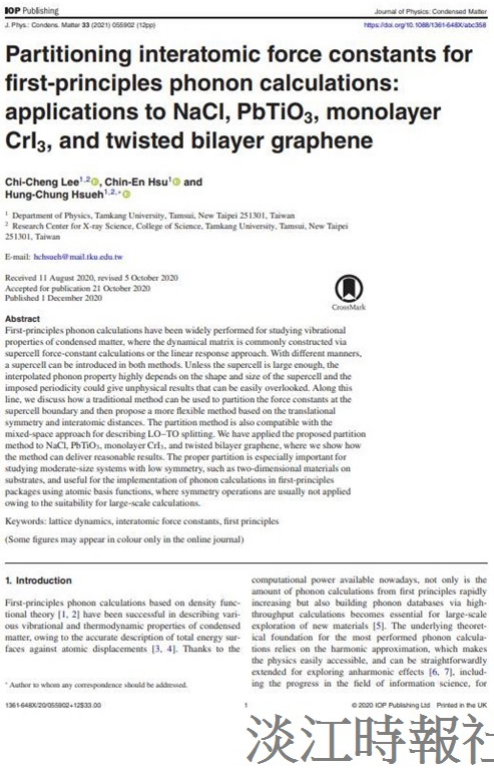
許誌恩說明已刊登的論文內容：「近年來，第一原理計算在諸多領域已取得相當大的成功，當中的聲子計算已實現在許多系統上，聲子計算有助於我們理解系統的晶體振動行為。透過分析固態系統中原子受力的關係修正，由於週期邊界條件與採用之單位晶胞尺度，造成聲子計算中力常數的錯誤，達到降低聲子計算所需之超晶胞大小與計算成本。」他坦言，是運用本校超高速電腦跑出來的數據，分析出結果。本校實驗室的設備幫助很大。

許誌恩表示，當第一篇研究論文刊登時，當時還是大學生，在履歷方面增加不少優勢，無論是就業或繼續求學，目前也與成大和台科大研究團隊合作其他實驗主題，「因淡江資源豐富，設備完善，實驗基本上都是利用學校電腦完成，同時有薛宏中和李啟正這樣優秀的教師，所以我選擇留在淡江。將來想到國外相關實驗室做博士後研究，繼續往學術研究道路邁進。」

2022/10/02

物理博一許誌恩連續發表論文登英美國際期刊。（攝影／江彥紳）



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**Partitioning interatomic force constants for first-principles phonon calculations: applications to NaCl, $PbTiO_3$, monolayer $CrI_3$, and twisted bilayer graphene**

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**Abstract**

First-principles phonon calculations have been widely performed for studying vibrational properties of condensed matter, where the dynamical matrix is commonly constructed via supercell force-constant calculations or the linear response approach. With different manners, a supercell can be introduced in both methods. Unless the supercell is large enough, the interpolated phonon property highly depends on the shape and size of the supercell and the imposed periodicity could give unphysical results that can be easily overlooked. Along this line, we discuss how a traditional method can be used to partition the force constants at the supercell boundary and then propose a more flexible method based on the translational symmetry and interatomic distances. The partition method is also compatible with the mixed-space approach for describing LO–TO splitting. We have applied the proposed partition method to NaCl, $PbTiO_3$, monolayer $CrI_3$, and twisted bilayer graphene, where we show how the method can deliver reasonable results. The proper partition is especially important for studying moderate-size systems with low symmetry, such as two-dimensional materials on substrates, and useful for the implementation of phonon calculations in first-principles packages using atomic basis functions, where symmetry operations are usually not applied owing to the suitability for large-scale calculations.

Keywords: lattice dynamics, interatomic force constants, first principles

(Some figures may appear in colour only in the online journal)

## 1. Introduction

First-principles phonon calculations based on density functional theory [1, 2] have been successful in describing various vibrational and thermodynamic properties of condensed matter, owing to the accurate description of total energy surfaces against atomic displacements [3, 4]. Thanks to the computational power available nowadays, not only is the amount of phonon calculations from first principles rapidly increasing but also building phonon databases via high-throughput calculations becomes essential for large-scale exploration of new materials [5]. The underlying theoretical foundation for the most performed phonon calculations relies on the harmonic approximation, which makes the physics easily accessible, and can be straightforwardly extended for exploring anharmonic effects [6, 7], including the progress in the field of information science, for

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物理系教授薛宏中、助理教授李啟正及理學院應用科學博一許誌恩，共同發表論文「新的原子震盪計算方法：以鹽與鉛鈦氧化薄層的原子為例」。（圖／許誌恩提供）