中研院、台大、清大研究團隊發現新拓樸材料,未來可望實現量子計算

中央研究院物理所莊天明博士與張嘉升博士所帶領的研究團隊與國立臺灣大學、國立清華大學合作，共同發現了超導性拓樸表面態存在於層狀材料 $PbTaSe_2$ 上。這項發現為研究拓樸超導體與未來的容錯性量子計算應用提供了一個優良的平臺。此一研究成果於 2016 年 11 月 23 日發表在美國科學促進會(American Association for the Advancement of Science; AAAS)出版之線上期刊「科學進展」(Science Advances)。

尋找物質的新狀態一直具有基礎科學和應用科技上的重要性。例如在磁性材料中，自旋的研究發現巨磁阻現象（2007 年諾貝爾獎）和硬碟的小型化。1980 年發現的量子霍爾效應（1985 年諾貝爾獎）和後續的拓樸能帶理論（今年諾貝爾獎）開闢了一個全新的拓樸相研究領域。拓樸絕緣體的理論預測和實驗確認是這個領域的重大進展。如同普通絕緣體一樣，拓樸絕緣體具有能隙可將共價帶與傳導帶的能帶分開。然而在材料的邊界處，拓樸絕緣體具有受拓樸保護的優異導電性。此邊界的導電性不易受到雜質影響，可以利用於高效的電子元件。

當拓樸絕緣體結合超導體時，理論上可以導致另一類重要的材料：拓樸超導體。 拓樸超導體的特徵在於能帶結構內的完整超導能隙和拓樸保護的無能隙表面態。在拓樸超導體中，一種尚未確認的費米子−馬約拉那(Majorana)費米子(此粒子為自身的反粒子)，會被束縛在如超導渦流這樣的拓樸缺陷，這樣的組合被預測會表現出非阿貝爾(non-Abelian)統計，因此可成為容錯性量子計算的基礎。在拓樸絕緣體中引入超導的最簡單方法是將其摻雜出超導性或於其上覆蓋 s-波超導體。然而，這兩種方法在技術上都是有挑戰性的，因為摻雜難以製造出均勻有序的材料，而在多層結構中製造出原子尺度下乾淨的界面也相當困難。

解決的方法是尋找適合的符合化學配比(stoichiometric)超導材料，在高於超導轉變溫度時，在費米面上展現出拓樸表面態，並且在超導態時，具有完整超導能隙。到目前為止，尚未有這種物質被發現。由中研院物理所的陳鵬仁博士和國立清華大學的鄭弘泰教授透過密度泛函計算研究層狀材料 $PbTaSe_2$ 的電子結構，發現其能滿足成為拓樸超導體的條件，他們的理論計算結果提供了實驗團隊清楚的動機與方向。材料由台大凝態中心的雷曼(Raman Sankar)博士和研究員周方正博士成功合成出高品質的單晶樣品，並由該中心研究員朱明文博士使用高解析的掃描穿透式電子顯微鏡確認詳細的晶體結構。$PbTaSe_2$ 的表面與電子結構則由台灣大學物理所博士生關旭佑、中研院物理所張嘉升博士和莊天明博士使用先進的自製掃描穿隧電子顯微鏡觀察原子尺度下電子的波函數變化，確認了理論預測中 $PbTaSe_2$ 的拓樸能帶的能譜特徵和超導特性。此研究成果為在符合化學配比的塊材中，首次發現到具有完整超導能隙的拓樸表面態。該團隊的成果展示 $PbTaSe_2$ 是一個值得重視的拓樸超導體候選材料。研究團隊下一步重點在於理解拓樸表面態進入超導態後的特性，以實現未來量子計算的目標。

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Scientists discover a material promising for future quantum computation

A research team led by Dr. Tien-Ming Chuang and Dr. Chia-Seng Chang at the Institute of Physics, Academia Sinica (AS), in collaboration with the researchers from National Taiwan University (NTU) and National Tsing Hua University (NTHU), has discovered the superconducting topological surface states in a layered material, $PbTaSe_2$. Their findings provide a great platform for the study of topological superconductivity toward the future application for the fault-tolerant quantum computing. Their results were published in the American Association for the Advancement of Science (AAAS) open access online magazine *Science Advances* on Nov 23, 2016.

The search of novel states of matter has always been of fundamental and technical importance. For example, the study of spin order in magnetic materials has led to the giant magnetoresistance (Nobel Prize in 2007) and the miniaturization of hard drives. The discovery of the quantum Hall effect in 1980 (Nobel Prize in 1985) and the subsequent development of topological band theory (Nobel Prize this year) have open a new field to the study of topological phases. The key development is the theoretical prediction and the experimental confirmation of topological insulators (TIs). A TI, like an ordinary insulator, has a bulk energy gap separating the highest valence band from the lowest conduction band. However, at the boundary, a TI has protected conducting states that are immune to impurities and useful for high performance electronics.

When a TI combined with superconductivity, it can theoretically lead to another important class of materials: topological superconductors (TSCs). TSCs are characterized by a full superconducting gap in the bulk and topologically protected gapless surface states. In a TSC, Majorana fermion, a hypothetical particle is its own anti-particle, is bound to a topological defect such as a superconducting vortex. Such combined objects are predicted to exhibit non-Abelian statistics and to form the basis of the fault-tolerant quantum computation. The simplest way to introduce superconductivity in a TI is by making it superconducting by doping or by coating a layer of s-wave superconductor. However, both approaches are technically challenging because it is difficult to make a homogenous doped material or a heterostructure with a clean interface.

The solution is to find a stoichiometric material that exhibits topological surface states at Fermi level in the normal state combined with fully gapped bulk superconductivity below T_C. So far, no such a bulk material is reported. Dr. Peng-Jen Chen from AS and Prof. Horng-Tay Jeng from NTHU found such requirements for a TSC are satisfied in a layered material, PbTaSe2 when studying its electronic structures by density functional theory. High quality single crystals are then synthesized by Dr. Raman Sankar and Dr. Fangcheng Chou at Center for Condensed Matter Sciences, NTU and the detailed crystal structure is confirmed by Dr. Ming-Wen Chu by using scanning transmission electron microscopy. By visualizing the electron wavefunction at atomic scale with the state-of-the-art home-built scanning tunneling microscopes, PhD student Syu-You Guan from NTU, Dr. Chia-Seng Chang and Dr. Tien-Ming Chuang from AS confirm the spectroscopic signature of the calculated topological band structures and superconducting properties in $PbTaSe_2$. The fully gapped superconducting topological surface state is reported for the first time in a stoichiometric bulk material. Their work shows $PbTaSe_2$ is a promising TSC candidate. The next step is to understand the nature of the superconducting topological surface state and to explore the novel topological superconducting phases towards future applications such as topological quantum computation.

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