「臺美奈米材料基礎科學研發共同合作研究計畫」
構想書徵求公告

(AFOSR-Taiwan NSTC Frontiers in Materials and Nanostructures: AI-Driven Discovery, Quantum Geometry, and Energy-Efficient Information Technologies)

一、計畫目標

臺灣與美國空軍之奈米材料基礎科學國際合作計畫，係為臺灣與美國研究人員提供交流與合作的平台，藉此能夠了解國際研究趨勢，及激發奈米科學最新技術，臺美雙方於 107 年以同步公開徵求與各自補助計畫的方式開始進行合作。現在公開徵求 116 年度新的三年期雙邊合作計畫。

本徵求公告之訂定日期時間係以臺灣時間為準。

二、申請條件

(一) 計畫主持人與共同主持人之資格，須符合「國科會補助專題研究計畫作業要點」相關辦法之規定。申請機構須為本會專題研究計畫之受補助機關。本計畫歸屬「雙邊協議專案型國際合作研究計畫」件數，不列入本會研究計畫件數的額度計算，惟以 2 件為限。

(二) 合作對象：**需包含 1 個(含)以上的美方研究人員。**該美方研究人員之服務機構，必須為美國學術研究單位或美國國防部(DoD)之受補助實驗室。如對美方研究人員資格有疑問，請與本案美方負責人員聯絡。美國空軍聯絡人 AFOSR Points of Contact (POC):
Lt Col Alexander Kamrud, alexander.kamrud.1@us.af.mil

三、徵求內容

The scientific focus will be on frontiers in materials and nanostructures that can advance science in the following concentration areas:

1. AI-driven materials discovery: We seek fundamental studies that integrate artificial intelligence, physics-based modeling, and experimental feedback to accelerate the discovery, synthesis, and understanding of solid-state materials, nanostructures, interfaces, molecules, and hybrid systems. Rather than purely data-driven screening or incremental database mining, this call emphasizes physically interpretable, uncertainty-aware, and experimentally validated approaches that reveal structure-property-function relationships across unexplored chemical, structural, and processing spaces. These efforts should enable predictive design of materials with targeted functionalities. Proposals are expected to align with one or more of the following core research tracks:

*** Physics-informed AI and quantum-level modeling:** Proposals may integrate machine learning with ab initio electronic-structure methods, quantum chemistry, molecular dynamics, many-body theory, or multiscale simulations to improve the accuracy, transferability, and efficiency of materials prediction. Emphasis should be placed on physically constrained and interpretable models that can predict key material properties while revealing the underlying structure–property relationships.

*** Predictive discovery, inverse design, and synthesis optimization:** Proposals may develop AI-guided approaches to identify stable or metastable materials, molecules, nanostructures, defects, interfaces, and heterostructures with targeted properties. Particular emphasis should be placed on uncertainty quantification, synthesis-aware design rules, closed-loop optimization, and experimentally testable predictions.

*** AI-enabled multiscale modeling of complex materials:** Proposals may leverage AI to bridge atomistic, mesoscale, and continuum descriptions of heterogeneous, disordered, interfacial, or nonequilibrium systems, including complex solids, molecular assemblies, low-dimensional heterostructures, multifunctional interfaces, and nanostructures whose properties emerge across multiple length and time scales.

2. Materials and nanostructures for energy-efficient electronic, photonic, and quantum information technologies: High energy demand driven by the rapid development of artificial intelligence represents a major challenge, making sustainable computing infrastructure highly desirable. We seek innovative materials and nanostructures that enable high-performance, low-power operation across computation, memory, data storage, optical interconnects, photonic or optoelectronic information processing, and emerging quantum information functionalities. Rather than system-level optimizations or conventional CMOS iterations, this call targets the synthesis, deterministic manipulation, and microscopic characterization of novel material phases, low-dimensional heterostructures, functional interfaces, and nanoscale photonic structures engineered to approach fundamental limits of energy-efficient information processing. Emphasis should be placed on material mechanisms, interfacial phenomena, nanoscale control, and experimentally measurable physical observables relevant to energy-efficient information processing.

3. Quantum geometry in solids:

Quantum geometry describes how electronic wavefunctions evolve in momentum space and governs emergent properties of solids, including topological and anomalous transport, nonlinear optical responses, and flat-band superconductivity. We seek scientific breakthrough to advance our understanding of quantum-geometric responses in materials. These efforts may guide the prediction and realization of new materials with enhanced emergent properties, potentially including robust high-temperature topological states. Proposals are expected to align with one or more of

the following core research tracks:

* **Advanced Experimental Methodologies to Resolve Quantum Geometry**: We seek new experimental methodologies to resolve quantum geometry in crystalline solids. Applicants are encouraged to extend these approaches to broad classes of quantum materials, such as topological materials, flat-band systems, moiré heterostructures, and superconductors. Methods that quantitatively isolate intrinsic Berry curvature and quantum metric contributions from conventional or extrinsic background responses, and benchmark experimental results against realistic first-principles or model calculations are desirable.

* **Novel Theoretical Frameworks Beyond DFT**: We seek new theoretical frameworks in which quantum geometry serves as a central descriptor of solids, complementing conventional band dispersion, symmetry, and Fermi-surface-based descriptions. Such frameworks should address realistic multiband, strongly correlated, disordered, and many-body systems, including, where relevant, interband mixing, electronic interactions, finite quasiparticle lifetimes, and non-translational configurations through Green's-function, diagrammatic, or kinetic approaches. They should clarify how quantum geometry governs nonlinear optical responses, transport, superconductivity, and collective phases, while providing experimentally testable criteria for separating intrinsic quantum-geometric effects from extrinsic contributions. The ultimate goal is to establish predictive design principles for quantum materials with enhanced novel functionalities.

四、申請流程與注意事項

1. 申請流程：本計畫申請區分「構想書(Pre-proposal/whitepapers)」及「完整計畫書(Full-proposal)」兩階段，由臺美雙方共同審查。**臺美合作雙方之申請人，必須個別向其補助機構(本會和美國空軍辦公室)依規定，分別同時提交內容相同之構想書內容，僅有一方提出申請，視同申請資格不符。**
2. 構想書格式：如附件，且每位申請人(/計畫主持人)**以申請 1 件為限**。
3. 計畫執行期限：民國 116 年 8 月 1 日至 119 年 7 月 31 日，共 3 年。
4. 經費編列注意事項：計畫主持人配合臺方與美方之相關規劃，進行年度或期末成果簡報致使產生業務費、國外差旅費等相關支出，由該計畫經費項下勻支，不得另案再向本會申請。
5. 構想書申請期限及送達方式：請循本會「專題研究計畫／(構想書計畫類別)臺美奈米材料基礎科學研發共同合作研究計畫構想書」線上申請方式作業，申請截止日期為 **115 年 10 月 2 日(含當日)**。

   臺方申請人於系統繳交送出後，顯示「計畫狀態：繳交送出(國科會)」。**確定個人繳交送出即完成申請，構想書階段不需要**經由申請機構之研發處送出，**不需要**申請機構造冊送國科會。

美方申請人必須依據附件二，依規定以電郵件方式，將構想書寄送 AFOSR Points of Contact (POC):
Lt Col Alexander Kamrud, alexander.kamrud.1@us.af.mil

6. 構想書審查方式：確定臺美雙方之申請人皆符合申請資格後，如有必要，申請人需至本會進行簡報並接受詢答，經通知未進行簡報者，其申請案不予推薦。本計畫經費係專款專用，無申覆機制。
7. 審查重點：
   - 研究內容必須具有創新性，著重於基礎科學原創性研究。
   - 雙邊合作的必要性。
   - 具發展潛力及未來性。
8. 構想書審查結果通知：構想書審查獲推薦者，將由本會自然處正式行文通知申請機構與申請人於期限內，提送完整計畫書(Full-proposal)，由申請機構造具名冊備函送達本會。通知日期依實際審查作業情形為準。

六、成果報告繳交、審查及評鑑

計畫主持人除依本會規範繳交研究成果等報告外，應於全程期末配合本會辦理成果審查等計畫評鑑作業。計畫主持人亦須配合臺方與美方之相關規劃，進行年度或期末成果簡報。

七、附件：可至本會自然處公告事項(https://www.nstc.gov.tw/nat/ch)下載
(1) 臺方構想書格式
(2) 美方徵求公告

八、聯絡資訊

本會自然處
奈米共同召集人 Dr. Tien-Ming Chuang(莊天明), chuangtm@gate.sinica.edu.tw
徐文章研究員或王心頎小姐，Tel：02-2737-7522。