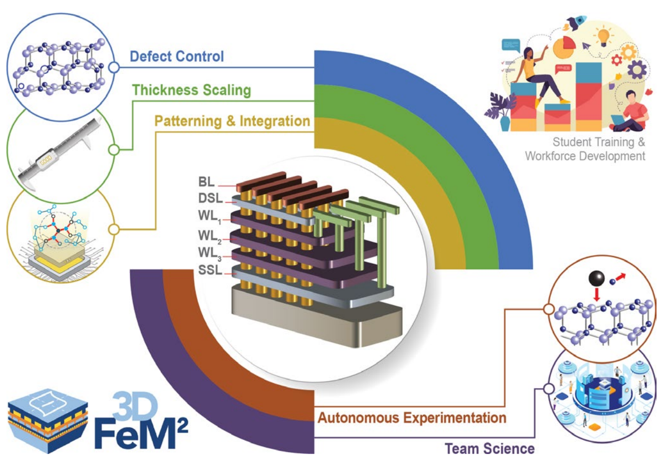
Center for 3 Dimensional Ferroelectric Microelectronics Manufacturing (3DFeM²)
EFRC Director: Susan Trolier-McKinstry
Lead Institution: The Pennsylvania State University
Class: 2020 – 2028

Mission Statement*: To integrate ferroelectric films at the required scale and reliability for 3D memory using next generation manufacturing practices.*

3DFeM² will develop three-dimensional (3D) non-volatile compute-in-memory technology that integrates novel ferroelectric materials into classical semiconductor manufacturing processes. This technology addresses tremendous societal needs for microelectronics that consume less energy without sacrificing performance, circumvents the end of Moore’s law in 2D scaling, and overcomes the “von Neumann bottleneck.”

3DFeM² will enable compute-in-memory chips and smart manufacturing by exploring the fundamental materials-physics of novel ferroelectricity and by developing a deeper scientific understanding of the underlying processes of 3D integration of ferroelectrics. Ultimately, the outcomes will enable a million-fold enhancement in interconnection between memory and logic, along with order of magnitude reductions in the energy cost to computation. ***This will be realized by developing the fundamental manufacturing science that assists the semiconductor transition to the fourth industrial revolution (Industry 4.0), a needed step for integrating robust ferroelectric materials that show outstanding properties throughout the device’s lifetime.*** The proposed 3D integrated ferroelectrics–deposited on geometrically complex surfaces with realistic back-end-of-the-line (BEOL) processing–will naturally fuse memory and computation and exploit the 3rd dimension, unleashing unprecedented capabilities for the next generation of computation and artificial intelligence. 3DFeM² will employ a data-driven co-design approach that overcomes the enormous obstacles for integrating new materials and realizing the lab-to-fab transition. We will implement digitalized processing instruments to generate large data sets, use physics-based machine learning (ML) to reduce experimental dimensionality, identify descriptors that can be monitored to assess properties in real time, establish autonomous experiments to expedite optimization, and develop digital twins that accelerate innovation through fast, cost-effective virtual experiments. In the process, 3DFeM² will transform semiconductor manufacturing practices while solving a critical societal energy challenge.



Vision for 3DFeM² in which fundamental materials science and processing science enable 3D ferroelectric memory for low power computing.

Ferroelectric fluorite and wurtzite crystals fundamentally change the device and integration landscape for ferroelectric microelectronics. *One of the key challenges for integrating new ferroelectrics is identification of the links between processing pathways and defects across length scales*. The role of defects must be understood early in the process of assessing new materials so potential failure modes can be identified prior to expensive scale-up in foundry settings. Key strategies for 3DFeM² are: ***i.*** innovations in materials and 3D structures that enable high-performance 3D ferroelectric random-access memory and high-density 3D ferroelectric NAND storage solutions; ***ii.*** materials-device-manufacturing co-design and co-optimization informed by ML models based on *in situ* processing and characterization data; and ***iii.*** digital twin creation of 3D ferroelectric memory to significantly accelerate the R&D to manufacturing pipeline.

The $3DFeM^2$ will target the following science goals: ***i.*** Understand how materials-chemistry design rules and processing boundary conditions regulate ferroelectricity in novel materials, ***ii.*** Understand and control ferroelectricity-enabling as well as the lifetime-limiting defects in next-generation ferroelectrics, ***iii.*** identify synthesis "descriptors," e.g., semi-empirical observables for defect chemistry, structure, and property evolution during material growth and etching, ***iv.*** characterize materials at previously inaccessible time and length scales, utilizing ML and *in situ* microscopy to identify phases, switching mechanisms, and scaling trends, ***v.*** enable autonomous workflows for optimized film growth and etching in 3D, ***vi.*** Generate device concepts best aligned with novel ferroelectric properties and target property metrics that maximize performance, and ***vii.*** establish a digital twin workflow that predicts performance and reliability with high accuracy based on device configuration, manufacturing process history and system-level operational characteristics.

$3DFeM^2$ will test two overarching hypotheses:

(1) Understanding domain walls, defects, interfaces, and intermediate switching structures of next-generation ferroelectrics at multiple length-scales will enable $3DFeM^2$ to engineer their coercive field, leakage current, and endurance characteristics and to discover superior ferroelectric formulations.

(2) Combining ML, *in situ* monitoring during synthesis and etch, and *in operando* device measurements will inform manufacturing science and expedite co-development of novel materials into 3D systems with high yields while creating a blueprint for future process innovations

Center for 3 Dimensional Ferroelectric Microelectronics Manufacturing ($3DFeM^2$)	
The Pennsylvania State University (lead)	Susan Trolier-McKinstry (Director) Betul Akkopru-Akgun, Venkatraman Gopalan, Thomas N. Jackson, Ying Liu, Jon-Paul Maria, Vijaykrishnan Narayanan, Darren Pagan, Clive Randall, Adri van Duin
Carnegie Mellon University	Elizabeth Dickey
Georgia Institute of Technology	Suman Datta, Lauren Garten, Asif Khan
The University of Notre Dame	Kai Ni
University of Maryland	A. Gilad Kusne, Ichiro Takeuchi
University of Pennsylvania	Andrew Rappe
University of Tennessee - Knoxville	Sergei Kalinin
University of Virginia	Patrick Hopkins, Jon Ihlefeld
Sandia National Laboratories	M. David Henry
Brookhaven National Laboratory	Judith Yang
Oak Ridge National Laboratory	Kyle Kelley, Rama Vasudevan

Contact: Susan Trolier-McKinstry, Director, STMcKinstry@psu.edu
814-863-8348, https://3dfem.psu.edu