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**Wei Zhang, Xi'an Jiaotong University**

**ABSTRACT**

**Chemical design principles for cache-type Sc-Sb-Te phase-change materials**

Nucleation is a critical issue in many scientific problems and technological processes, and is difficult to control due to its stochastic nature. The stochasticity of crystal nucleation poses challenges that limit technological advances. Here we highlight one such case: in phase change materials (PCMs, one prototypical example being Ge2Sb2Te5, GST), the stochastic nucleation rate is too low to enable sub-nanosecond memory writing for the build-up of universal memory hierarchy. In this talk, I will show how to engineer the intrinsic nucleation properties of PCMs to achieve sub-ns writing speed via ab initio materials design. The alloy design was based on density functional theory (DFT) simulations and quantum chemistry bonding analysis to single out the optimal element Sc to incorporate into Sb2Te3. As speculated, the Sc additions in the resultant Sc0.2Sb2Te3 (SST), are shown to stabilize the four-fold rings and cubes (crystalline precursors) by forming geometrically-matched and high-strength ScTe bonds, drastically reducing the stochasticity of the incubation process. These robust crystalline precursors serve as the centers for subsequent rapid nucleation and crystal growth, as revealed by ab initio molecular dynamics (AIMD) simulations. This discovery made it possible to reach a record-high writing speed, ~700 picoseconds, even in a conventional phase change memory device without the need of pre-programming treatment or complex device design. [1-2]

References:

[1] F. Rao,\* K. Ding, Y.-X. Zhou, Y. Zheng, M. Xia, S. Lv, Z. Song,\* S. Feng, I. Ronneberger, R. Mazzarello, W. Zhang,\* E. Ma, Reducing the stochasticity of crystal nucleation to enable subnanosecond memory writing. Science 358, 1423-1427 (2017).

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**BIO**

Dr. Wei Zhang is a professor in the School of Materials Science and Engineering at Xi’an Jiaotong University, where he is supported by the Youth Thousand Talents Program of China and the Young Talent Support Plan of Xi'an Jiaotong University.