Abstract Submitted
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Terminating Surface Electromigration at the Source[1] KIRK BEVAN, McGill University / Oak Ridge National Laboratory, WENGUANG ZHU, University of Tennessee / Oak Ridge National Laboratory, HONG GUO, McGill University, ZHENYU ZHANG, Oak Ridge National Laboratory / University of Tennessee / University of Science and Technology of China — Through an extensive search across the periodic table utilizing first-principles density functional theory, we have established a general elemental trend for determining electromigration inhibiting impurities on the technologically important Cu(111) surface – the dominant diffusion pathway in modern nanoelectronics interconnects. Unrecognized thus far, such inhibitors are characterized by energetically favoring (and binding strongly at) the kink sites of step edges. These properties are determined to generally reside in elements that form strong covalent bonds with substrate metal atoms. This finding sheds new light on the possibility of halting surface electromigration via kink blocking impurities.

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