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First principles investigation of polymer-ceramic interfaces and composites V. RANJAN, L. YU, M. BUONGIORNO NARDELLI, J. BERNHOLC, North Carolina State University — Composite structures with high-k dielectrics are important future technologies for high-performance capacitors. We perform generalized-gradient approximation calculations to study interfacial properties of ceramic-polymer composites, focusing in particular on the strength of polymer adhesion to ceramic surfaces. Our results show that several polymers of interest do not bind directly to the ceramic. However, it is possible to functionalize the surface so that polymer attachment occurs. We present various possibilities for attachment to ceramic surfaces, which should lead to the formation of stable composites.

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