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General methodology for creating improved polymeric dielectrics[1] MAYANK MISRA, MANISH AGARWAL, DANIEL SINKOVITS, SANAT KUMAR, Columbia University — We use molecular dynamics and density functional theory to show that the addition of a small number of polar -OH groups to an apolar, hydrocarbon polymer increases the dielectric constant by a factor of 2, but without substantially increasing the dielectric loss. While these results, which are in good agreement with experiments, point to a specific route to creating improved capacitors, more generally, these results suggest that improved polymeric based dielectric materials can be designed by incorporating polar groups on the chain, but only those whose relaxations can be substantially slowed due to cooperative effects, e.g., through long-lived hydrogen bonds.

[1]Multidisciplinary University Research Initiative (MURI)

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