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Holes influence the mutation spectrum of human mitochondrial DNA. MARTHA VILLAGRAN, JOHN MILLER, University of Houston, Dept. of Physics Texas Ctr. for Superconductivity — Mutations drive evolution and disease, showing highly non-random patterns of variant frequency *vs.* nucleotide position. We use computational DNA hole spectroscopy [M.Y. Suarez-Villagran & J.H. Miller, Sci. Rep. 5, 13571 (2015)] to reveal sites of enhanced hole probability in selected regions of human mitochondrial DNA. A hole is a mobile site of positive charge created when an electron is removed, for example by radiation or contact with a mutagenic agent. The hole spectra are quantum mechanically computed using a two-stranded tight binding model of DNA. We observe significant correlation between spectra of hole probabilities and of genetic variation frequencies from the MITOMAP database. These results suggest that hole-enhanced mutation mechanisms exert a substantial, perhaps dominant, influence on mutation patterns in DNA. One example is where a trapped hole induces a hydrogen bond shift, known as tautomerization, which then triggers a base-pair mismatch during replication. Our results deepen overall understanding of sequence specific mutation rates, encompassing both hotspots and cold spots, which drive molecular evolution.

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