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Spontaneous oscillation of current in fullerene molecular junctions CHAO-CHENG KAUN, RYAN JORN, TAMAR SEIDEMAN, Department of Chemistry, Northwestern University — We study the correlated phenomena of resonant conduction and current-driven dynamics in Au-C₆₀-Au molecular junctions from first principles. A significant resonant component of the transmission gives rise to vibrations of the C₆₀ center of mass between the electrodes [C.-C. Kaun and T. Seideman, PRL 94, 226801 (2005)]. An interesting interplay between conduction channels of different symmetries and different degrees of spatial localization results in strong dependence of the transmission on the location of the fullerene within the junction. The distance-dependence, in turn, leads to oscillating current in the THz regime. Rotation of the C₆₀ about its axis likewise markedly modifies the transmission characteristics.

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