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First Principles study of the formation of molecular junctions: benzenethiolate on Au (111) YONGDUO LIU, VIDVUDS OZOLINS — We perform density functional calculations to study the formation mechanism of benzenethiolate molecular junctions on the Au (111) surface. Specifically, we investigate the geometry change and the mechanical properties of the metal-molecule contact when it is under stretching. It is found that by pulling up the thiolate molecule from Au (111), one Au surface atom can be converted to an adatom. And moreover, if the stretching is continued, another Au atom would successively be pulled up to form a two-atom bridge between the Au (111) and the sulfur end group. Based on these findings, we propose a mechanism to the formation of pyramidal molecular junctions: benzenethiolate on Au (111).

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