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Polymerization of methane in the deep Earth[1] LEONARDO SPANU, Department of Chemistry UC Davis, DAVIDE DONADIO, MPI for Polymer Research; Department of Chemistry UC Davis, DETLEF HOHL, Shell Global Solutions Inc. Houston, TX, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore CA, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis — Determining physical and chemical properties of carbon fluids at high pressure and temperature is a key step towards understanding carbon reservoirs and fluxes in the deep Earth. The stability of carbon-hydrogen systems at depth greater than few thousands meters is poorly understood and the abiogenic hypothesis on the synthesis of higher hydrocarbon (HCs) in the Earth mantle remains controversial. We have used ab initio molecular dynamics simulations to investigate the formation of higher HCs from dissociation of pure methane, and of methane in contact with carbon surfaces and transition metals, in a range of pressure of $2 - 30$ GPa and temperature T=$800 - 4,000$ K [1]. We present results on the range of stability of pure methane and discuss how the interaction with transition metals or carbon deposits (graphite and diamond) affects the formation of higher HCs.

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