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**Methane under pressure: dissociation reactions from ab initio simulation**[1] DETLEF HOHL, Shell International Exploration and Production, Rijswijk, The Netherlands, LEONARDO SPANU, DAVIDE DONADIO, Department of Chemistry, University of California at Davis, Davis, 95616 CA, ERIC SCHWEGLER, Lawrence Livermore Natl. Lab. Livermore, CA 94551 USA, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California at Davis, Davis, 95616 CA, GIULIA GALLI, Chemistry Department UC Davis and Physics Department UC Davis, Davis 95616 CA — Using ab initio molecular dynamics [1], we have investigated the stability of methane under pressure up to $\sim$ 24 GPa and in the temperature range $2 - 4000$ K, studied in recent diamond anvil cell experiments [2]. In particular, we have explored the possible formation of alkanes from methane dissociation. We have calculated structural and vibrational properties, and compared the relative stability of several hydrocarbons mixtures. Our results show that the temperature is the main driving force for methane dissociation, with pressure enhancing the formation of higher hydrocarbons, at temperatures where dissociation is observed. [1] Qbox code: http://eslab.ucsvais.edu [2] A. Kolesnikov, Kutcherov VG. and Goncharov AF. *Nature Geoscience* , (2009) **8** (566-570)

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