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18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 3101)

Saturday 14 January 2017

Session:	Functionals	and efficient	approaches

- Leonardo Building - Budinich Lecture Hall (09:00-11:35)

time	title	presenter
09:00	Introduction to the session	
09:05	Advances in semi-empirical density functionals for molecules and materials	M. HEAD-GORDON
	Electron correlation from the adiabatic-connection-fluctuation-dissipation-theorem approach for a multireference wavefunction	K. PERNAL
	Strongly Constrained and Appropriately Normed (SCAN) Semilocal Density Functional: Accurate and Efficient for Structures and Energies of Diversely-Bonded Materials	J. SUN
10:35	Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation and Applications	M. GOVONI
11:05	Concluding Remarks	