

# SAIP 2011



Contribution ID : 22

## **Algebraic density functionals**

Friday 15 Jul 2011 at 11:45 (00h30')

### **Content :**

A systematic strategy for the algebraic calculation of density functionals consists in coding information about the density and the energy into polynomials of the degrees of freedom of the wave functions. Density functionals and Kohn-Sham potentials are then obtained by standard elimination procedures of such degrees of freedom between the polynomials. Numerical examples illustrate the formalism.

### **Level (Hons, MSc, PhD, other)? :**

Other

### **Consider for a student award (Yes / No)? :**

No

### **Short Paper :**

Yes

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**Session classification** : Theoretical

**Track classification** : Track G - Theoretical and Computational Physics

**Type** : Oral Presentation