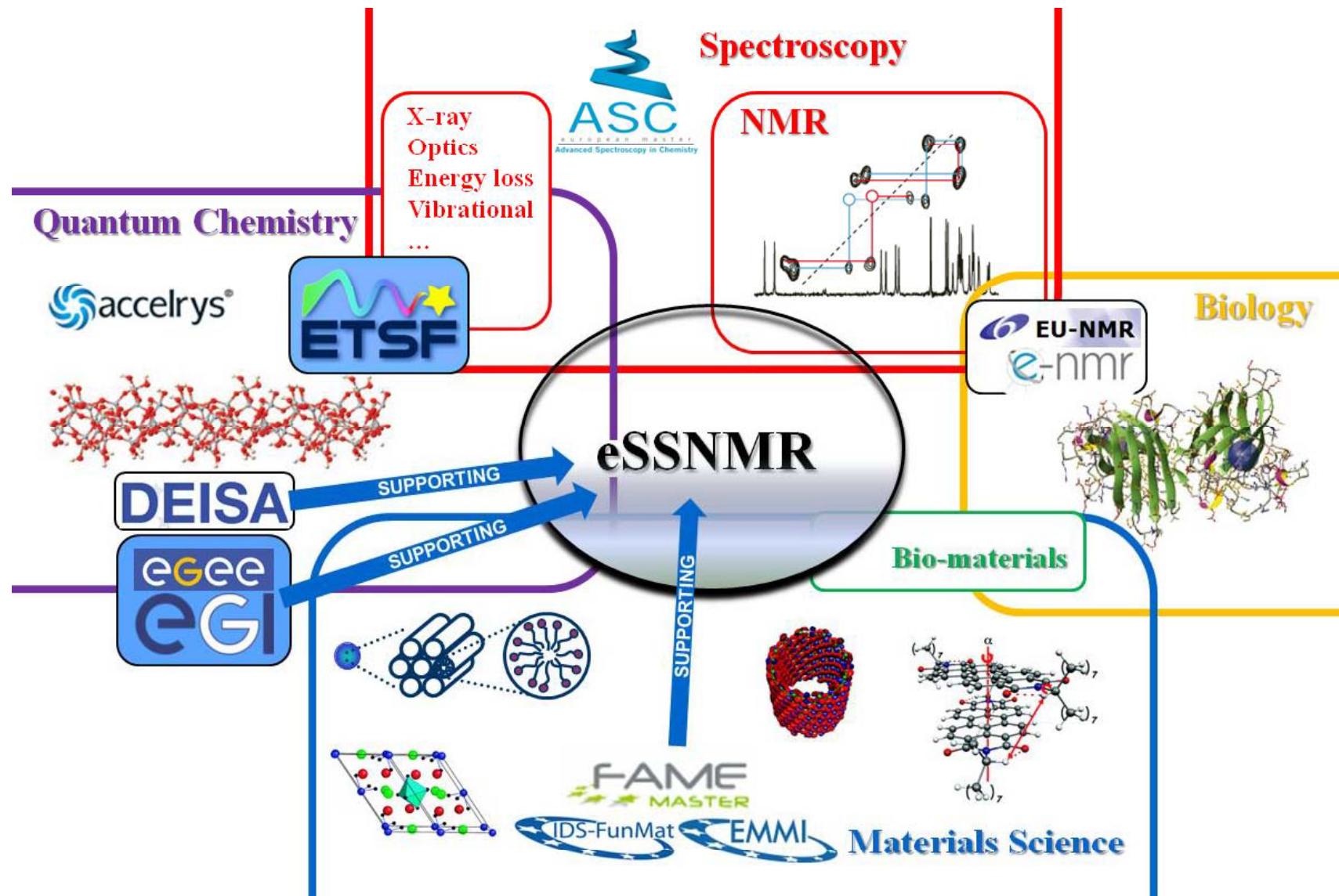


# Materials by Solid State NMR – modelling & ab-initio computing



# eSSNMR - State of the Art

DM

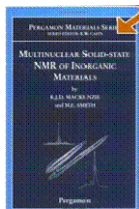


- *dmfit* : fitting software for end users (Materials Science & Engineering)  
~850 registered users with downloads since 2008 (~2000 since 2002)  
670 citations (~80/year) - 8<sup>th</sup> best cited paper in the 10 last years (Engineering) - ISI

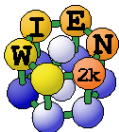
TV



- *SIMPSON* : *in silico* NMR spectrometer  
~500 Users (NMR Spectroscopists)  
>500 citations (~60/year) - ISI  
Discussion group



- *Multinuclear Solid-State NMR of Materials*  
review of > 1 000 published experimental data  
no existing on line database



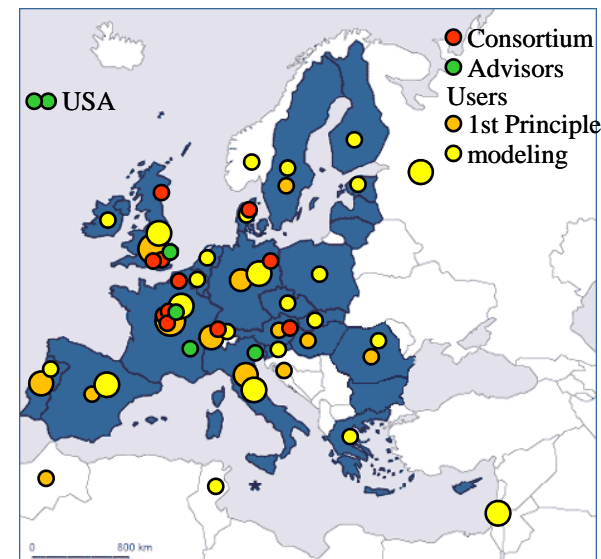
- *Wien2k* : All electron DFT (LAPW)  
~1500 registered users – forum  
423 papers dealing with NMR  
User's meeting & Discussion group

JRY



**CASTEP**

- *GIPAW (CASTEP & PWscf)* : Pseudopotentials  
commercial & open-source  
seminal paper : 158 citations (>40/year 2008-2009)  
User's meeting, training & discussion groups



**European / International leading software and expertise  
yet scattered pieces**

# eSSNMR - Pert Diagram

