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The screenshot displays the Materials Studio 2017 interface. The main window shows a CASTEP SCF Energy plot with Energy (eV) on the y-axis (ranging from -6500 to -6900) and Iteration on the x-axis (ranging from 1 to 5). The energy values are approximately: Iteration 1: -6500 eV, Iteration 2: -6850 eV, Iteration 3: -6850 eV, Iteration 4: -6850 eV, Iteration 5: -6850 eV. A molecular model of a protein is shown in the background. Several windows are open, including 'About Materials Studio' (version 17.1.0.48), 'CASTEP Calculation' (Task: Energy, Functional: GGA/PBE), and 'Lalanine CASTEP Energy (2)\Status.txt' (Job Name: l_alanine_NMR, type of calculation: Magnetic Resonance, plane wave basis set cut-off: 571.4000 eV, Magnetic Resonance Property: Chemical shielding + using Functional: Perdew Burke Ernzerhof). The 'Jobs' window at the bottom shows a table of running jobs:

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
l_alanin...	MXOAI	localhost:...	CASTEP	running	1/5/2017 ...	\l_alanine...	

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