Buildings in the United States are responsible for more than 40% of the primary energy and 70% of electricity usage and greatly in CO2 emission by about 39%, more than any other sector including transportation and industry sectors. This energy consumption is expected to grow mainly due to increasing trends in new buildings construction. Rising energy prices alongside with energy independencies, limited resources, and climate change have made the current situation even worse. An Energy Efficient (EE) building is able to reduce the heating and cooling load significantly compared with a code compliant building. Furthermore, integrating renewable energy sources in the building energy portfolio could drive the building’s grid reliance further down. Such buildings that are able to passively save and actively produce energy are called Net Zero Energy Buildings (NZEB). Despite all new energy efficient technologies, reaching NZEB is challenging due to high first cost of super-efficient measures and renewable energy sources as well as integration of the newly on-site generated electricity to the grid. Achieving NZEB without looking at its surrounding environment may result in sub-optimal solutions. Currently, 95% of American households own a car, and with the help of newly introduced Vehicle to Home (V2H) technologies, building, vehicle, renewable energy sources, and ecological environment can work together as a techno-ecological system to fulfill the requirement of an NZEB ecosystem. Due to the great flexibility of electric vehicles (EVs) and plug-in hybrid electric vehicles (PHEVs) in interacting with the power grid, they will play a significant role in the future of the power system. This dissertation aims to utilizes the application of vehicle to home technology to reach NZEB by developing two new models in two phases; the macro based excel model (NZEB-VBA) and agent based model (NZEB-ABM). In the first step, an optimization analysis is performed to select the best design alternatives for an energy-efficient building under the relevant economic and environmental constraints. Next, solar photovoltaic sources are used to supply the building's remaining energy demand and thereby minimize the building's grid reliance. Finally, Vehicle to Home technology is coupled with the renewable energy source as a substitute for power from the grid. In the second phase of the study, it is tried to more focus on the dynamic interaction of different components of the system with each other. Although the general procedure is the same but, the whole modeling will be taken place in a different environment. The results indicate that, with the help of energy-efficient design features and a properly developed algorithm to draw electricity from EV and solar energy, it is possible to reduce the required electricity from the power grid by 59% compared to a standard energy-efficient building and by as much as 90% compared to a typical code-compliant building, thereby reducing the electricity cost by 1.55 times compared to the conventional method of drawing grid electricity which can compensate the installation costs of solar panels and other technologies necessary for a net zero energy building.